



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:49 AM UTC

PDB ID : 8SLW / pdb_00008slw
EMDB ID : EMD-40581
Title : Cryo-EM structure of the rat TRPM5 channel in 2mM calcium, high-4
Authors : Karuppan, S.; Schrag, L.G.; Jara-Oseguera, A.; Zubcevic, L.
Deposited on : 2023-04-24
Resolution : 4.20 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

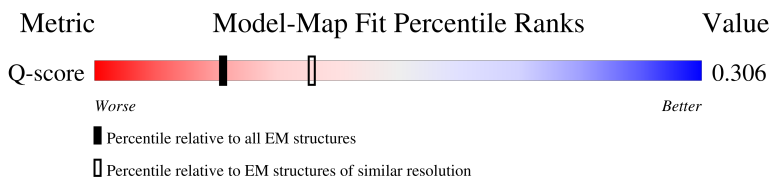
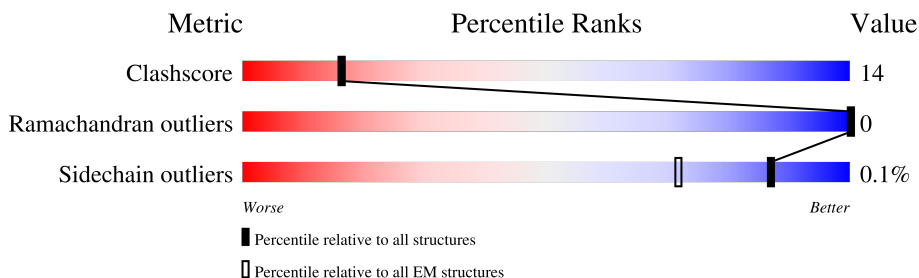
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1169	 60% 19% 21%
1	B	1169	 60% 19% 21%
1	C	1169	 60% 18% 21%
1	D	1169	 60% 18% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25964 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily M member 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	921	Total	C	N	O	S	0	0
			6489	4189	1149	1130	21		
1	B	921	Total	C	N	O	S	0	0
			6489	4189	1149	1130	21		
1	C	921	Total	C	N	O	S	0	0
			6489	4189	1149	1130	21		
1	D	921	Total	C	N	O	S	0	0
			6489	4189	1149	1130	21		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A455XI77
A	-9	ASP	-	expression tag	UNP A0A455XI77
A	-8	TYR	-	expression tag	UNP A0A455XI77
A	-7	LYS	-	expression tag	UNP A0A455XI77
A	-6	ASP	-	expression tag	UNP A0A455XI77
A	-5	ASP	-	expression tag	UNP A0A455XI77
A	-4	ASP	-	expression tag	UNP A0A455XI77
A	-3	ASP	-	expression tag	UNP A0A455XI77
A	-2	LYS	-	expression tag	UNP A0A455XI77
A	-1	LEU	-	expression tag	UNP A0A455XI77
A	0	GLU	-	expression tag	UNP A0A455XI77
A	156	ALA	-	insertion	UNP A0A455XI77
A	157	GLN	-	insertion	UNP A0A455XI77
B	-10	MET	-	initiating methionine	UNP A0A455XI77
B	-9	ASP	-	expression tag	UNP A0A455XI77
B	-8	TYR	-	expression tag	UNP A0A455XI77
B	-7	LYS	-	expression tag	UNP A0A455XI77
B	-6	ASP	-	expression tag	UNP A0A455XI77
B	-5	ASP	-	expression tag	UNP A0A455XI77
B	-4	ASP	-	expression tag	UNP A0A455XI77
B	-3	ASP	-	expression tag	UNP A0A455XI77

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	LYS	-	expression tag	UNP A0A455XI77
B	-1	LEU	-	expression tag	UNP A0A455XI77
B	0	GLU	-	expression tag	UNP A0A455XI77
B	156	ALA	-	insertion	UNP A0A455XI77
B	157	GLN	-	insertion	UNP A0A455XI77
C	-10	MET	-	initiating methionine	UNP A0A455XI77
C	-9	ASP	-	expression tag	UNP A0A455XI77
C	-8	TYR	-	expression tag	UNP A0A455XI77
C	-7	LYS	-	expression tag	UNP A0A455XI77
C	-6	ASP	-	expression tag	UNP A0A455XI77
C	-5	ASP	-	expression tag	UNP A0A455XI77
C	-4	ASP	-	expression tag	UNP A0A455XI77
C	-3	ASP	-	expression tag	UNP A0A455XI77
C	-2	LYS	-	expression tag	UNP A0A455XI77
C	-1	LEU	-	expression tag	UNP A0A455XI77
C	0	GLU	-	expression tag	UNP A0A455XI77
C	156	ALA	-	insertion	UNP A0A455XI77
C	157	GLN	-	insertion	UNP A0A455XI77
D	-10	MET	-	initiating methionine	UNP A0A455XI77
D	-9	ASP	-	expression tag	UNP A0A455XI77
D	-8	TYR	-	expression tag	UNP A0A455XI77
D	-7	LYS	-	expression tag	UNP A0A455XI77
D	-6	ASP	-	expression tag	UNP A0A455XI77
D	-5	ASP	-	expression tag	UNP A0A455XI77
D	-4	ASP	-	expression tag	UNP A0A455XI77
D	-3	ASP	-	expression tag	UNP A0A455XI77
D	-2	LYS	-	expression tag	UNP A0A455XI77
D	-1	LEU	-	expression tag	UNP A0A455XI77
D	0	GLU	-	expression tag	UNP A0A455XI77
D	156	ALA	-	insertion	UNP A0A455XI77
D	157	GLN	-	insertion	UNP A0A455XI77

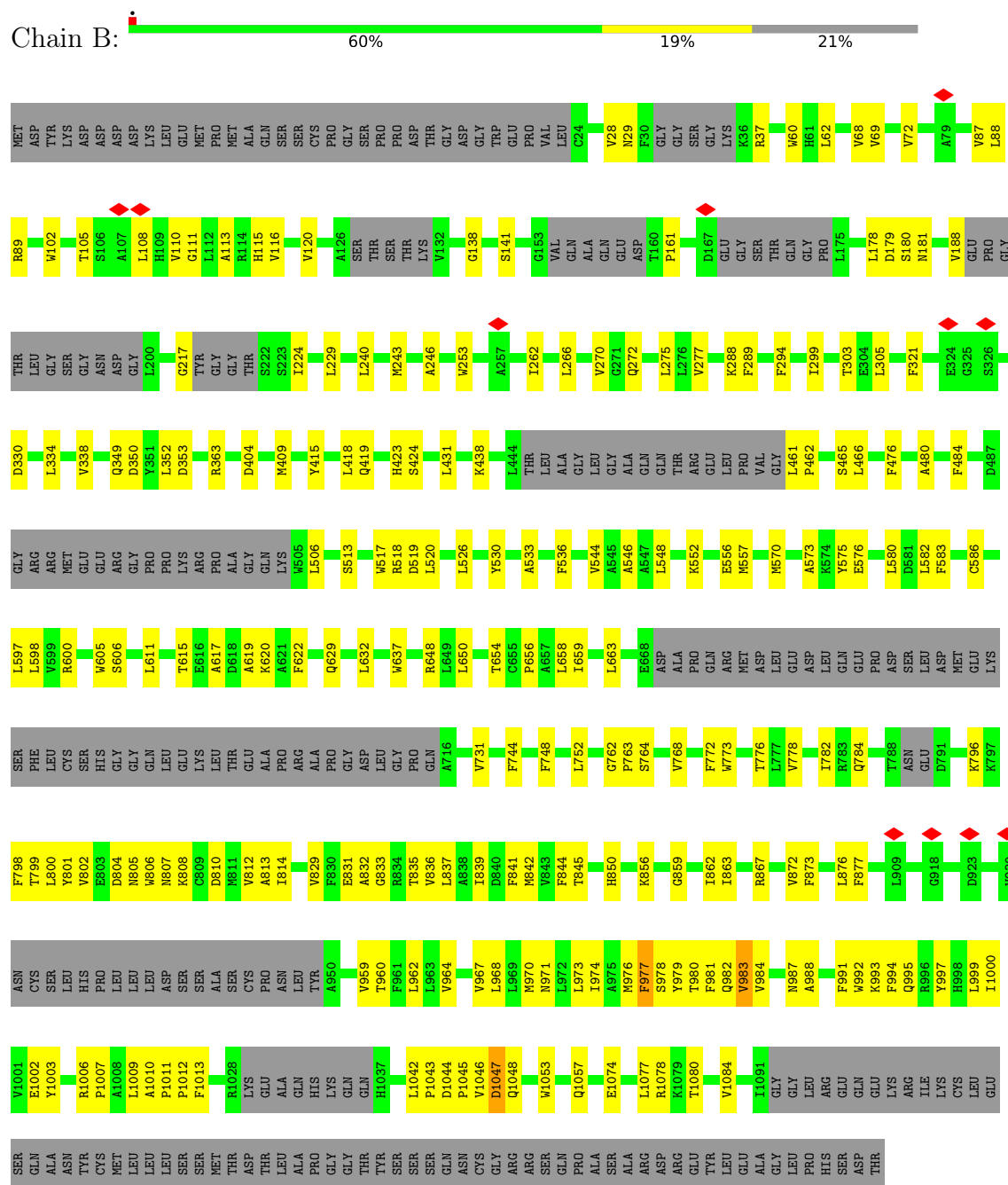
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

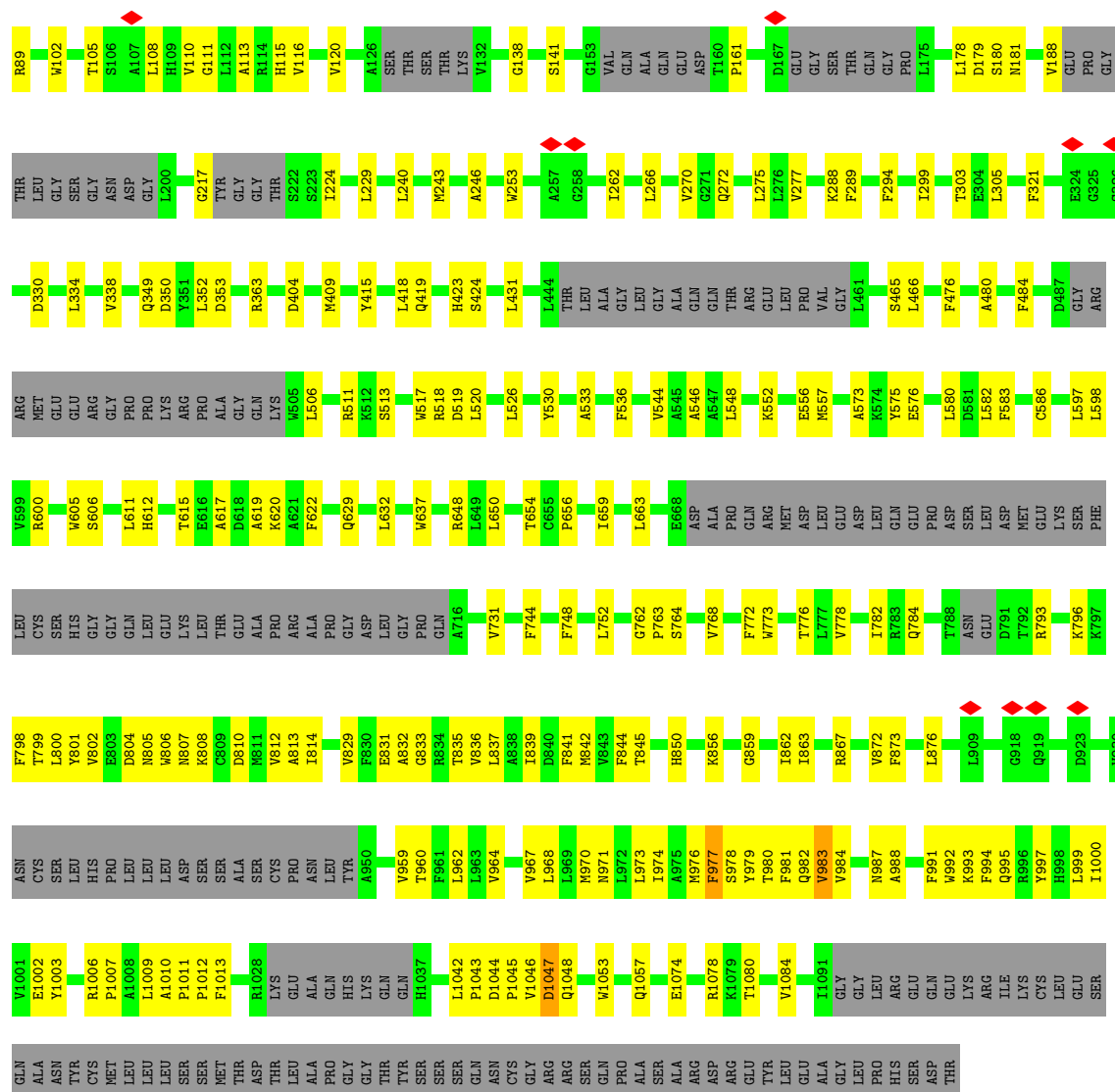
Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Ca 2 2	0
2	B	2	Total Ca 2 2	0
2	C	2	Total Ca 2 2	0
2	D	2	Total Ca 2 2	0

GLN
ALA
ASN
TYR
CYS
MET
LEU
LEU
LEU
SER
SER
THR
MET
THR
MET
ASP
THR
ALA
SER
PRO
CYS
GLY
GLY
THR
TYR
SER
SER
SER
SER
GLN
ASN
CYS
GLY
GLY
ARG
ARG
SER
GLN
VAL
PRO
ALA
ALA
SER
ALA
ARG
ASP
ARG
GLY
GLY
SER
TYR
LEU
LEU
GLU
ALA
GLY
LEU
LEU
PRO
HIS
SER
ASP
THR

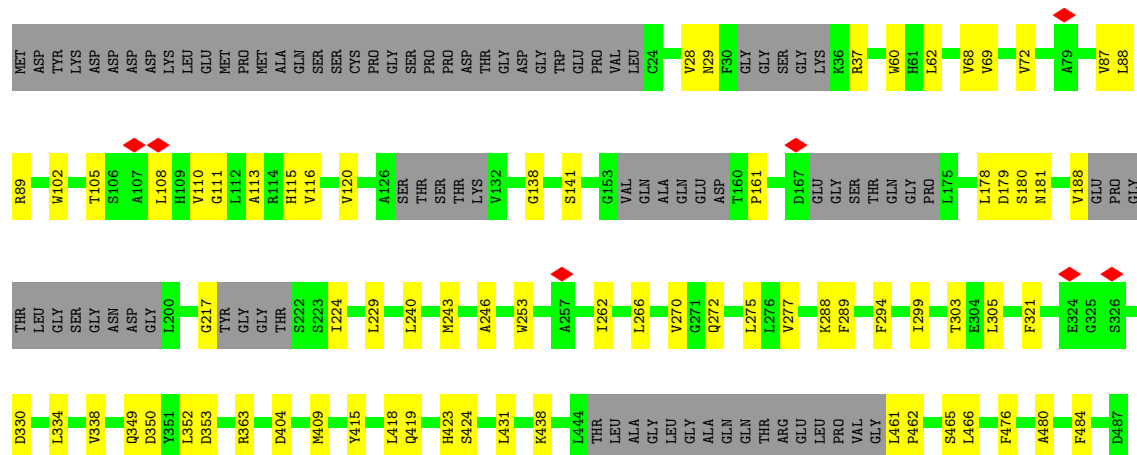
- Molecule 1: Transient receptor potential cation channel subfamily M member 5

Chain B:





• Molecule 1: Transient receptor potential cation channel subfamily M member 5



ASN	TYR	CYS	MET	LEU	LEU	LEU	LEU	LEU	SER	SER	MET	THR	ASP	THR	LEU	ALA	GLN	HIS	GLY	LYS	GLN	THR	TYR	SER	SER	SER	GLN	ASN	CYS	GLY	ALA	PRO	GLN	GLY	ALA	TYR	ASN	TYR	ASP	THR	LEU	GLU	GLY	GLY	LEU	PRO	HIS	ASP	THR					
Y1003	R1006	P1007	A1008	A1009	A1010	P1011	P1012	F1013	R1028	LYS	GLU	ALA	GLN	HIS	GLY	LYS	GLN	GLN	H1037	L1042	P1043	D1044	P1045	D1046	D1047	Q1048	W1053	Q1057	E1074	R1078	K1079	T1080	V1084	I1091	GLY	GLY	LEU	PRO	HIS	ASP	THR	LEU	GLU	GLU	GLN	LYS	LYS	ILE	CYS	LEU	GLU	SER	GLN	ALA
SER	LEU	HIS	PRO	LEU	LEU	ASP	SER	ALA	SER	CYS	PRO	ASN	LEU	TYR	A950	V959	T960	F961	L962	L963	V964	V967	L968	L969	N970	N971	L972	L973	1974	A975	N976	F977	S978	1979	F981	Q982	V983	V984	N987	A988	F991	Q992	K993	F994	Q995	R996	Y997	H998	L999	11000	V1001	E1002		
F798	T799	Y801	V802	E803	D804	N805	W806	N807	K808	C809	D810	H811	V812	A813	T814	V829	F830	E831	A832	G833	R834	T835	V836	L837	I839	D840	F841	F844	T845	H850	K856	G859	I862	I863	R867	V872	F873	L876	L909	G918	D923	V930	ASN	CYS										
SER	PHE	LEU	CYS	SER	HIS	GLY	GLN	LEU	GLU	LYS	LEU	THR	GLU	ALA	ARG	ALA	PRO	GLY	ASP	LEU	GLY	PRO	GLN	A716	V731	F744	F748	L752	G762	P763	S764	V768	I772	W773	T776	L777	V778	I782	R783	Q784	T788	ASN	GLU	D791	K796	K797								
L597	ARG	ARG	MET	GLU	GLU	ARG	GLY	PRO	PRO	LYS	ARG	PRO	ALA	GLY	GLN	LYS	W505	L506	R511	K512	S513	W517	R518	D519	L520	L526	Y530	A533	F536	V544	A545	A546	A547	L548	K552	E556	M557	A573	K574	Y575	E576	L580	D581	L582	F583	C586								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	44520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.721	Depositor
Minimum map value	-0.428	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	403.2, 403.2, 403.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	1/6633 (0.0%)	0.51	4/9082 (0.0%)
1	B	0.29	2/6633 (0.0%)	0.51	4/9082 (0.0%)
1	C	0.29	2/6633 (0.0%)	0.50	4/9082 (0.0%)
1	D	0.29	2/6633 (0.0%)	0.51	4/9082 (0.0%)
All	All	0.29	7/26532 (0.0%)	0.51	16/36328 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1047	ASP	C-N	5.16	1.40	1.33
1	D	1047	ASP	C-N	5.16	1.40	1.33
1	B	977	PHE	C-O	-5.10	1.18	1.24
1	D	977	PHE	C-O	-5.09	1.18	1.24
1	A	1047	ASP	C-N	5.09	1.40	1.33
1	B	1047	ASP	C-N	5.07	1.40	1.33
1	C	977	PHE	C-O	-5.02	1.18	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	973	LEU	O-C-N	6.46	128.73	122.07
1	A	973	LEU	O-C-N	6.46	128.72	122.07
1	D	973	LEU	O-C-N	6.42	128.69	122.07
1	B	973	LEU	O-C-N	6.41	128.68	122.07
1	D	987	ASN	N-CA-C	5.89	117.38	111.07
1	B	987	ASN	N-CA-C	5.86	117.34	111.07
1	C	987	ASN	N-CA-C	5.84	117.32	111.07
1	A	987	ASN	N-CA-C	5.78	117.26	111.07
1	C	974	ILE	N-CA-C	5.39	116.16	110.72
1	D	974	ILE	N-CA-C	5.37	116.14	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	974	ILE	N-CA-C	5.35	116.12	110.72
1	B	974	ILE	N-CA-C	5.33	116.11	110.72
1	D	983	VAL	N-CA-C	-5.10	105.52	110.42
1	A	983	VAL	N-CA-C	-5.08	105.54	110.42
1	C	983	VAL	N-CA-C	-5.06	105.56	110.42
1	B	983	VAL	N-CA-C	-5.04	105.58	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6489	0	5718	180	0
1	B	6489	0	5718	177	0
1	C	6489	0	5718	175	0
1	D	6489	0	5718	173	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
All	All	25964	0	22872	694	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (694) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ARG:NH1	1:D:115:HIS:HB3	1.22	1.45
1:C:89:ARG:NH1	1:C:115:HIS:HB3	1.22	1.44
1:A:89:ARG:NH1	1:A:115:HIS:HB3	1.22	1.43
1:B:89:ARG:NH1	1:B:115:HIS:HB3	1.22	1.42
1:D:863:ILE:CG2	1:D:988:ALA:HB1	1.63	1.29
1:B:863:ILE:CG2	1:B:988:ALA:HB1	1.63	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:863:ILE:CG2	1:C:988:ALA:HB1	1.63	1.28
1:A:863:ILE:CG2	1:A:988:ALA:HB1	1.63	1.27
1:B:89:ARG:HH12	1:B:115:HIS:CB	1.57	1.17
1:D:89:ARG:HH12	1:D:115:HIS:CB	1.57	1.17
1:B:863:ILE:HG21	1:B:988:ALA:HB1	1.23	1.16
1:C:89:ARG:HH12	1:C:115:HIS:CB	1.57	1.15
1:A:89:ARG:HH12	1:A:115:HIS:CB	1.57	1.15
1:C:863:ILE:HG21	1:C:988:ALA:HB1	1.22	1.14
1:A:863:ILE:HG21	1:A:988:ALA:HB1	1.23	1.13
1:D:863:ILE:HG21	1:D:988:ALA:HB1	1.22	1.12
1:C:978:SER:O	1:C:982:GLN:HG3	1.54	1.08
1:D:978:SER:O	1:D:982:GLN:HG3	1.54	1.07
1:A:978:SER:O	1:A:982:GLN:HG3	1.54	1.06
1:B:978:SER:O	1:B:982:GLN:HG3	1.54	1.05
1:B:89:ARG:NH1	1:B:115:HIS:CB	2.17	1.04
1:D:89:ARG:NH1	1:D:115:HIS:CB	2.17	1.04
1:A:970:MET:HE1	1:C:970:MET:HE1	1.38	1.04
1:C:89:ARG:NH1	1:C:115:HIS:CB	2.17	1.04
1:A:89:ARG:NH1	1:A:115:HIS:CB	2.17	0.99
1:A:89:ARG:CZ	1:A:115:HIS:HB3	2.01	0.91
1:C:89:ARG:CZ	1:C:115:HIS:HB3	2.01	0.90
1:B:89:ARG:CZ	1:B:115:HIS:HB3	2.01	0.90
1:A:970:MET:HE1	1:C:970:MET:CE	2.01	0.89
1:D:89:ARG:CZ	1:D:115:HIS:HB3	2.01	0.89
1:B:976:MET:O	1:B:980:THR:CB	2.24	0.85
1:C:977:PHE:O	1:C:981:PHE:N	2.10	0.85
1:A:976:MET:O	1:A:980:THR:CB	2.24	0.84
1:D:976:MET:O	1:D:980:THR:CB	2.24	0.84
1:C:976:MET:O	1:C:980:THR:CB	2.24	0.84
1:D:977:PHE:O	1:D:981:PHE:CB	2.26	0.84
1:A:977:PHE:O	1:A:981:PHE:CB	2.26	0.84
1:B:976:MET:O	1:B:980:THR:N	2.12	0.83
1:D:977:PHE:O	1:D:981:PHE:N	2.10	0.83
1:A:977:PHE:O	1:A:981:PHE:N	2.10	0.83
1:B:977:PHE:O	1:B:981:PHE:N	2.10	0.83
1:B:977:PHE:O	1:B:981:PHE:CB	2.26	0.83
1:C:977:PHE:O	1:C:981:PHE:CB	2.26	0.83
1:A:976:MET:O	1:A:980:THR:N	2.12	0.83
1:D:863:ILE:CG2	1:D:988:ALA:CB	2.56	0.82
1:C:976:MET:O	1:C:980:THR:N	2.12	0.82
1:D:976:MET:O	1:D:980:THR:N	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:ILE:CG2	1:A:988:ALA:CB	2.56	0.79
1:A:859:GLY:HA3	1:A:992:TRP:HE1	1.48	0.79
1:D:859:GLY:HA3	1:D:992:TRP:HE1	1.48	0.79
1:B:859:GLY:HA3	1:B:992:TRP:HE1	1.48	0.78
1:C:859:GLY:HA3	1:C:992:TRP:HE1	1.48	0.78
1:C:863:ILE:HG21	1:C:988:ALA:CB	2.12	0.77
1:A:978:SER:O	1:A:982:GLN:CG	2.34	0.76
1:C:863:ILE:CG2	1:C:988:ALA:CB	2.56	0.76
1:B:863:ILE:CG2	1:B:988:ALA:CB	2.56	0.76
1:D:978:SER:O	1:D:982:GLN:CG	2.34	0.75
1:B:978:SER:O	1:B:982:GLN:CG	2.34	0.75
1:A:970:MET:HE1	1:B:970:MET:HE1	1.68	0.75
1:D:863:ILE:HG21	1:D:988:ALA:CB	2.12	0.74
1:A:863:ILE:HG21	1:A:988:ALA:CB	2.12	0.73
1:A:999:LEU:HD23	1:A:999:LEU:C	2.14	0.73
1:D:999:LEU:C	1:D:999:LEU:HD23	2.14	0.73
1:C:544:VAL:HG11	1:C:597:LEU:HD21	1.70	0.73
1:A:415:TYR:CE1	1:A:513:SER:HA	2.24	0.73
1:C:999:LEU:HD23	1:C:999:LEU:C	2.14	0.73
1:B:415:TYR:CE1	1:B:513:SER:HA	2.24	0.72
1:C:978:SER:O	1:C:982:GLN:CG	2.34	0.72
1:B:999:LEU:C	1:B:999:LEU:HD23	2.14	0.71
1:C:415:TYR:CE1	1:C:513:SER:HA	2.24	0.71
1:A:863:ILE:HG22	1:A:988:ALA:HB1	1.71	0.71
1:D:1042:LEU:CB	1:D:1043:PRO:CD	2.68	0.71
1:D:1043:PRO:HD2	1:D:1046:VAL:HB	1.73	0.71
1:C:1043:PRO:HD2	1:C:1046:VAL:HB	1.73	0.71
1:D:415:TYR:CE1	1:D:513:SER:HA	2.24	0.71
1:A:1043:PRO:HD2	1:A:1046:VAL:HB	1.73	0.71
1:A:1042:LEU:CB	1:A:1043:PRO:CD	2.68	0.71
1:B:415:TYR:HE1	1:B:513:SER:HA	1.56	0.71
1:B:1043:PRO:HD2	1:B:1046:VAL:HB	1.73	0.71
1:C:1042:LEU:CB	1:C:1043:PRO:CD	2.68	0.71
1:B:1042:LEU:CB	1:B:1043:PRO:CD	2.68	0.70
1:D:415:TYR:HE1	1:D:513:SER:HA	1.56	0.69
1:B:863:ILE:HG21	1:B:988:ALA:CB	2.12	0.69
1:A:415:TYR:HE1	1:A:513:SER:HA	1.56	0.69
1:B:620:LYS:HG2	1:B:994:PHE:CD1	2.28	0.69
1:C:620:LYS:HG2	1:C:994:PHE:CD1	2.28	0.69
1:C:970:MET:HE1	1:D:970:MET:HE1	1.75	0.69
1:B:1042:LEU:CB	1:B:1043:PRO:HD2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LEU:CB	1:A:1043:PRO:HD2	2.23	0.68
1:C:431:LEU:CD1	1:C:526:LEU:HB3	2.23	0.68
1:C:1042:LEU:CB	1:C:1043:PRO:HD2	2.23	0.68
1:D:431:LEU:CD1	1:D:526:LEU:HB3	2.23	0.68
1:D:620:LYS:HG2	1:D:994:PHE:CD1	2.28	0.68
1:A:431:LEU:CD1	1:A:526:LEU:HB3	2.23	0.68
1:A:620:LYS:HG2	1:A:994:PHE:CD1	2.28	0.68
1:D:1042:LEU:CB	1:D:1043:PRO:HD2	2.23	0.68
1:C:415:TYR:HE1	1:C:513:SER:HA	1.56	0.68
1:D:68:VAL:HG12	1:D:102:TRP:HB2	1.76	0.68
1:B:68:VAL:HG12	1:B:102:TRP:HB2	1.76	0.68
1:A:970:MET:CE	1:B:970:MET:HE1	2.23	0.67
1:B:431:LEU:CD1	1:B:526:LEU:HB3	2.23	0.67
1:C:68:VAL:HG12	1:C:102:TRP:HB2	1.76	0.67
1:C:580:LEU:HD21	1:C:622:PHE:HA	1.77	0.67
1:D:863:ILE:HG22	1:D:988:ALA:HB1	1.71	0.67
1:D:580:LEU:HD21	1:D:622:PHE:HA	1.77	0.67
1:B:970:MET:HE1	1:D:970:MET:HE1	1.76	0.66
1:A:68:VAL:HG12	1:A:102:TRP:HB2	1.76	0.66
1:A:580:LEU:HD21	1:A:622:PHE:HA	1.77	0.66
1:A:629:GLN:HE21	1:A:993:LYS:HD3	1.61	0.66
1:B:580:LEU:HD21	1:B:622:PHE:HA	1.77	0.66
1:B:863:ILE:HG22	1:B:988:ALA:HB1	1.71	0.66
1:C:859:GLY:HA3	1:C:992:TRP:NE1	2.11	0.66
1:B:859:GLY:HA3	1:B:992:TRP:NE1	2.11	0.66
1:C:629:GLN:HE21	1:C:993:LYS:HD3	1.61	0.66
1:B:629:GLN:HE21	1:B:993:LYS:HD3	1.61	0.65
1:D:859:GLY:HA3	1:D:992:TRP:NE1	2.11	0.65
1:A:859:GLY:HA3	1:A:992:TRP:NE1	2.11	0.64
1:A:970:MET:CE	1:C:970:MET:CE	2.74	0.64
1:C:1044:ASP:N	1:C:1045:PRO:HD2	2.13	0.64
1:B:1044:ASP:N	1:B:1045:PRO:HD2	2.13	0.64
1:D:629:GLN:HE21	1:D:993:LYS:HD3	1.61	0.64
1:A:1044:ASP:N	1:A:1045:PRO:HD2	2.13	0.64
1:C:863:ILE:HG22	1:C:988:ALA:HB1	1.71	0.63
1:D:1044:ASP:N	1:D:1045:PRO:HD2	2.13	0.63
1:C:217:GLY:HA3	1:C:224:ILE:H	1.65	0.61
1:A:217:GLY:HA3	1:A:224:ILE:H	1.65	0.61
1:B:272:GLN:HB2	1:B:275:LEU:HD13	1.83	0.61
1:D:217:GLY:HA3	1:D:224:ILE:H	1.65	0.61
1:A:272:GLN:HB2	1:A:275:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:798:PHE:O	1:D:802:VAL:HG23	2.02	0.60
1:B:970:MET:CE	1:D:970:MET:HE1	2.31	0.60
1:D:272:GLN:HB2	1:D:275:LEU:HD13	1.83	0.60
1:B:217:GLY:HA3	1:B:224:ILE:H	1.65	0.60
1:C:89:ARG:HH12	1:C:115:HIS:HB3	0.69	0.59
1:A:798:PHE:O	1:A:802:VAL:HG23	2.02	0.59
1:B:798:PHE:O	1:B:802:VAL:HG23	2.02	0.59
1:C:798:PHE:O	1:C:802:VAL:HG23	2.02	0.59
1:C:272:GLN:HB2	1:C:275:LEU:HD13	1.83	0.59
1:D:465:SER:OG	1:D:506:LEU:HD21	2.03	0.59
1:A:465:SER:OG	1:A:506:LEU:HD21	2.03	0.58
1:B:277:VAL:O	1:B:303:THR:OG1	2.21	0.58
1:C:1080:THR:O	1:C:1084:VAL:HG23	2.02	0.58
1:A:1080:THR:O	1:A:1084:VAL:HG23	2.02	0.58
1:B:1080:THR:O	1:B:1084:VAL:HG23	2.02	0.58
1:D:1080:THR:O	1:D:1084:VAL:HG23	2.02	0.58
1:B:465:SER:OG	1:B:506:LEU:HD21	2.03	0.58
1:C:240:LEU:HD13	1:C:262:ILE:HD11	1.86	0.58
1:C:465:SER:OG	1:C:506:LEU:HD21	2.03	0.58
1:D:240:LEU:HD13	1:D:262:ILE:HD11	1.86	0.58
1:D:744:PHE:HB2	1:D:773:TRP:CE2	2.39	0.58
1:C:1074:GLU:O	1:C:1078:ARG:HD3	2.04	0.58
1:A:1074:GLU:O	1:A:1078:ARG:HD3	2.04	0.57
1:C:752:LEU:HD11	1:C:837:LEU:HB3	1.86	0.57
1:C:967:VAL:O	1:C:971:ASN:CB	2.52	0.57
1:C:744:PHE:HB2	1:C:773:TRP:CE2	2.39	0.57
1:B:240:LEU:HD13	1:B:262:ILE:HD11	1.86	0.57
1:D:1074:GLU:O	1:D:1078:ARG:HD3	2.04	0.57
1:B:1074:GLU:O	1:B:1078:ARG:HD3	2.04	0.57
1:C:772:PHE:O	1:C:776:THR:HG23	2.05	0.57
1:D:835:THR:O	1:D:839:ILE:HG12	2.05	0.57
1:A:835:THR:O	1:A:839:ILE:HG12	2.05	0.57
1:A:744:PHE:HB2	1:A:773:TRP:CE2	2.39	0.57
1:C:835:THR:O	1:C:839:ILE:HG12	2.05	0.57
1:B:744:PHE:HB2	1:B:773:TRP:CE2	2.39	0.57
1:C:520:LEU:HB3	1:C:536:PHE:CE2	2.40	0.57
1:A:752:LEU:HD11	1:A:837:LEU:HB3	1.86	0.57
1:A:240:LEU:HD13	1:A:262:ILE:HD11	1.86	0.56
1:B:835:THR:O	1:B:839:ILE:HG12	2.05	0.56
1:D:772:PHE:O	1:D:776:THR:HG23	2.05	0.56
1:B:772:PHE:O	1:B:776:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:LYS:O	1:C:800:LEU:HG	2.05	0.56
1:D:520:LEU:HB3	1:D:536:PHE:CE2	2.40	0.56
1:A:772:PHE:O	1:A:776:THR:HG23	2.05	0.56
1:D:29:ASN:H	1:D:161:PRO:HB3	1.71	0.56
1:D:752:LEU:HD11	1:D:837:LEU:HB3	1.86	0.56
1:D:978:SER:O	1:D:982:GLN:N	2.37	0.56
1:B:520:LEU:HB3	1:B:536:PHE:CE2	2.40	0.56
1:C:744:PHE:HB2	1:C:773:TRP:CZ2	2.41	0.56
1:D:744:PHE:HB2	1:D:773:TRP:CZ2	2.41	0.56
1:A:29:ASN:H	1:A:161:PRO:HB3	1.71	0.56
1:D:796:LYS:O	1:D:800:LEU:HG	2.05	0.56
1:B:752:LEU:HD11	1:B:837:LEU:HB3	1.86	0.56
1:C:29:ASN:H	1:C:161:PRO:HB3	1.71	0.56
1:A:520:LEU:HB3	1:A:536:PHE:CE2	2.40	0.56
1:A:796:LYS:O	1:A:800:LEU:HG	2.05	0.56
1:A:744:PHE:HB2	1:A:773:TRP:CZ2	2.41	0.55
1:A:970:MET:CE	1:C:970:MET:HE3	2.35	0.55
1:B:796:LYS:O	1:B:800:LEU:HG	2.05	0.55
1:B:29:ASN:H	1:B:161:PRO:HB3	1.71	0.55
1:B:744:PHE:HB2	1:B:773:TRP:CZ2	2.41	0.55
1:D:748:PHE:HE2	1:D:841:PHE:HB2	1.72	0.55
1:A:748:PHE:HE2	1:A:841:PHE:HB2	1.72	0.55
1:B:28:VAL:O	1:B:37:ARG:HA	2.07	0.55
1:B:349:GLN:HA	1:B:352:LEU:HD13	1.89	0.55
1:C:629:GLN:NE2	1:C:993:LYS:HB3	2.22	0.55
1:A:349:GLN:HA	1:A:352:LEU:HD13	1.89	0.55
1:B:978:SER:O	1:B:982:GLN:N	2.37	0.55
1:C:28:VAL:O	1:C:37:ARG:HA	2.07	0.55
1:B:629:GLN:NE2	1:B:993:LYS:HB3	2.22	0.54
1:D:629:GLN:NE2	1:D:993:LYS:HB3	2.22	0.54
1:A:28:VAL:O	1:A:37:ARG:HA	2.07	0.54
1:A:629:GLN:NE2	1:A:993:LYS:HB3	2.22	0.54
1:C:748:PHE:HE2	1:C:841:PHE:HB2	1.72	0.54
1:D:349:GLN:HA	1:D:352:LEU:HD13	1.89	0.54
1:C:349:GLN:HA	1:C:352:LEU:HD13	1.89	0.54
1:A:873:PHE:O	1:A:876:LEU:HG	2.08	0.54
1:D:832:ALA:O	1:D:836:VAL:HG23	2.08	0.54
1:D:873:PHE:O	1:D:876:LEU:HG	2.08	0.54
1:B:873:PHE:O	1:B:876:LEU:HG	2.08	0.54
1:D:28:VAL:O	1:D:37:ARG:HA	2.07	0.54
1:C:873:PHE:O	1:C:876:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:PHE:HE2	1:B:841:PHE:HB2	1.72	0.53
1:B:810:ASP:O	1:B:814:ILE:HG12	2.09	0.53
1:B:832:ALA:O	1:B:836:VAL:HG23	2.08	0.53
1:A:978:SER:O	1:A:982:GLN:N	2.37	0.53
1:B:1053:TRP:NE1	1:B:1057:GLN:HE21	2.07	0.53
1:C:832:ALA:O	1:C:836:VAL:HG23	2.08	0.53
1:A:810:ASP:O	1:A:814:ILE:HG12	2.09	0.53
1:A:991:PHE:O	1:A:995:GLN:N	2.36	0.53
1:C:1053:TRP:NE1	1:C:1057:GLN:HE21	2.07	0.53
1:D:810:ASP:O	1:D:814:ILE:HG12	2.09	0.53
1:A:476:PHE:CZ	1:A:557:MET:HG2	2.44	0.53
1:B:476:PHE:CZ	1:B:557:MET:HG2	2.44	0.53
1:A:409:MET:HG3	1:A:517:TRP:CH2	2.44	0.53
1:C:480:ALA:O	1:C:605:TRP:C	2.52	0.53
1:A:831:GLU:O	1:A:835:THR:HG23	2.09	0.52
1:C:810:ASP:O	1:C:814:ILE:HG12	2.09	0.52
1:A:480:ALA:O	1:A:605:TRP:C	2.52	0.52
1:C:330:ASP:OD2	1:C:363:ARG:NH2	2.42	0.52
1:D:409:MET:HG3	1:D:517:TRP:CH2	2.44	0.52
1:B:409:MET:HG3	1:B:517:TRP:CH2	2.44	0.52
1:B:960:THR:O	1:B:964:VAL:HG12	2.09	0.52
1:C:418:LEU:HD11	1:C:519:ASP:HB3	1.91	0.52
1:D:480:ALA:O	1:D:605:TRP:C	2.52	0.52
1:D:831:GLU:O	1:D:835:THR:HG23	2.09	0.52
1:A:330:ASP:OD2	1:A:363:ARG:NH2	2.42	0.52
1:A:832:ALA:O	1:A:836:VAL:HG23	2.08	0.52
1:B:418:LEU:HD11	1:B:519:ASP:HB3	1.91	0.52
1:D:330:ASP:OD2	1:D:363:ARG:NH2	2.42	0.52
1:D:960:THR:O	1:D:964:VAL:HG12	2.09	0.52
1:A:108:LEU:CB	1:A:178:LEU:HD13	2.40	0.52
1:C:831:GLU:O	1:C:835:THR:HG23	2.09	0.52
1:B:330:ASP:OD2	1:B:363:ARG:NH2	2.42	0.52
1:B:480:ALA:O	1:B:605:TRP:C	2.52	0.52
1:B:178:LEU:HD12	1:B:179:ASP:H	1.75	0.52
1:C:1010:ALA:HB3	1:C:1013:PHE:HD2	1.75	0.52
1:A:960:THR:O	1:A:964:VAL:HG12	2.09	0.52
1:A:1053:TRP:NE1	1:A:1057:GLN:HE21	2.07	0.52
1:B:266:LEU:O	1:B:270:VAL:HG23	2.10	0.52
1:B:831:GLU:O	1:B:835:THR:HG23	2.09	0.52
1:C:108:LEU:CB	1:C:178:LEU:HD13	2.40	0.52
1:C:409:MET:HG3	1:C:517:TRP:CH2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:THR:O	1:C:964:VAL:HG12	2.09	0.52
1:D:1053:TRP:NE1	1:D:1057:GLN:HE21	2.07	0.52
1:B:808:LYS:O	1:B:812:VAL:HG23	2.10	0.52
1:C:476:PHE:CZ	1:C:557:MET:HG2	2.44	0.52
1:D:476:PHE:CZ	1:D:557:MET:HG2	2.44	0.52
1:C:266:LEU:O	1:C:270:VAL:HG23	2.10	0.52
1:D:762:GLY:H	1:D:763:PRO:HD2	1.75	0.52
1:D:991:PHE:O	1:D:995:GLN:N	2.36	0.52
1:A:178:LEU:HD12	1:A:179:ASP:H	1.75	0.51
1:B:1010:ALA:HB3	1:B:1013:PHE:HD2	1.75	0.51
1:C:762:GLY:H	1:C:763:PRO:HD2	1.75	0.51
1:D:178:LEU:HD12	1:D:179:ASP:H	1.75	0.51
1:D:418:LEU:HD11	1:D:519:ASP:HB3	1.91	0.51
1:A:1010:ALA:HB3	1:A:1013:PHE:HD2	1.75	0.51
1:D:808:LYS:O	1:D:812:VAL:HG23	2.10	0.51
1:A:418:LEU:HD11	1:A:519:ASP:HB3	1.91	0.51
1:A:808:LYS:O	1:A:812:VAL:HG23	2.10	0.51
1:C:978:SER:O	1:C:982:GLN:N	2.37	0.51
1:A:762:GLY:H	1:A:763:PRO:HD2	1.76	0.51
1:B:108:LEU:CB	1:B:178:LEU:HD13	2.40	0.51
1:B:762:GLY:H	1:B:763:PRO:HD2	1.76	0.51
1:D:611:LEU:O	1:D:615:THR:HG23	2.11	0.51
1:A:60:TRP:HB3	1:A:62:LEU:HD13	1.93	0.51
1:B:60:TRP:HB3	1:B:62:LEU:HD13	1.93	0.51
1:C:808:LYS:O	1:C:812:VAL:HG23	2.10	0.51
1:D:108:LEU:CB	1:D:178:LEU:HD13	2.40	0.51
1:D:266:LEU:O	1:D:270:VAL:HG23	2.10	0.51
1:B:611:LEU:O	1:B:615:THR:HG23	2.11	0.51
1:A:796:LYS:O	1:A:799:THR:OG1	2.27	0.51
1:C:611:LEU:O	1:C:615:THR:HG23	2.11	0.51
1:D:60:TRP:HB3	1:D:62:LEU:HD13	1.93	0.51
1:A:266:LEU:O	1:A:270:VAL:HG23	2.10	0.50
1:A:277:VAL:O	1:A:303:THR:OG1	2.21	0.50
1:C:60:TRP:HB3	1:C:62:LEU:HD13	1.93	0.50
1:C:178:LEU:HD12	1:C:179:ASP:H	1.75	0.50
1:A:611:LEU:O	1:A:615:THR:HG23	2.11	0.50
1:D:546:ALA:O	1:D:548:LEU:N	2.44	0.50
1:B:546:ALA:O	1:B:548:LEU:N	2.44	0.50
1:C:546:ALA:O	1:C:548:LEU:N	2.44	0.50
1:A:419:GLN:HG2	1:A:423:HIS:CE1	2.46	0.50
1:C:179:ASP:OD1	1:C:180:SER:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ALA:O	1:A:548:LEU:N	2.44	0.50
1:A:1009:LEU:HD22	1:A:1013:PHE:HB3	1.94	0.50
1:D:1010:ALA:HB3	1:D:1013:PHE:HD2	1.75	0.50
1:B:419:GLN:HG2	1:B:423:HIS:CE1	2.46	0.50
1:C:1009:LEU:HD22	1:C:1013:PHE:HB3	1.94	0.50
1:D:419:GLN:HG2	1:D:423:HIS:CE1	2.46	0.50
1:B:431:LEU:HD13	1:B:526:LEU:HB3	1.92	0.50
1:B:89:ARG:HH12	1:B:115:HIS:HB3	0.69	0.49
1:B:179:ASP:OD1	1:B:180:SER:N	2.45	0.49
1:B:804:ASP:OD1	1:B:805:ASN:N	2.45	0.49
1:D:89:ARG:HH12	1:D:115:HIS:HB3	0.69	0.49
1:D:480:ALA:O	1:D:606:SER:CB	2.60	0.49
1:C:480:ALA:O	1:C:606:SER:CB	2.60	0.49
1:A:804:ASP:OD1	1:A:805:ASN:N	2.45	0.49
1:C:419:GLN:HG2	1:C:423:HIS:CE1	2.46	0.49
1:A:778:VAL:O	1:A:782:ILE:HG13	2.13	0.49
1:B:778:VAL:O	1:B:782:ILE:HG13	2.13	0.49
1:D:804:ASP:OD1	1:D:805:ASN:N	2.45	0.49
1:B:415:TYR:CE1	1:B:513:SER:CA	2.94	0.49
1:A:415:TYR:CE1	1:A:513:SER:CA	2.94	0.49
1:B:424:SER:O	1:B:424:SER:OG	2.27	0.49
1:C:465:SER:OG	1:C:466:LEU:N	2.46	0.49
1:D:431:LEU:HD13	1:D:526:LEU:HB3	1.92	0.49
1:B:991:PHE:O	1:B:995:GLN:N	2.36	0.49
1:C:141:SER:HA	1:C:188:VAL:HB	1.95	0.49
1:C:804:ASP:OD1	1:C:805:ASN:N	2.45	0.49
1:A:480:ALA:O	1:A:606:SER:CB	2.60	0.49
1:B:1009:LEU:HD22	1:B:1013:PHE:HB3	1.94	0.49
1:C:964:VAL:O	1:C:968:LEU:CB	2.61	0.49
1:D:1009:LEU:HD22	1:D:1013:PHE:HB3	1.94	0.49
1:A:424:SER:O	1:A:424:SER:OG	2.27	0.49
1:C:796:LYS:O	1:C:799:THR:OG1	2.27	0.49
1:D:141:SER:HA	1:D:188:VAL:HB	1.95	0.49
1:D:598:LEU:HG	1:D:611:LEU:HD21	1.95	0.49
1:A:179:ASP:OD1	1:A:180:SER:N	2.45	0.48
1:B:598:LEU:HG	1:B:611:LEU:HD21	1.95	0.48
1:C:778:VAL:O	1:C:782:ILE:HG13	2.13	0.48
1:A:243:MET:O	1:A:246:ALA:HB3	2.13	0.48
1:C:415:TYR:CE1	1:C:513:SER:CA	2.94	0.48
1:D:179:ASP:OD1	1:D:180:SER:N	2.45	0.48
1:A:116:VAL:O	1:A:120:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:SER:HA	1:B:188:VAL:HB	1.95	0.48
1:A:598:LEU:HG	1:A:611:LEU:HD21	1.95	0.48
1:D:465:SER:OG	1:D:466:LEU:N	2.46	0.48
1:A:999:LEU:C	1:A:999:LEU:CD2	2.85	0.48
1:B:465:SER:OG	1:B:466:LEU:N	2.46	0.48
1:D:650:LEU:O	1:D:654:THR:HG23	2.13	0.48
1:A:89:ARG:HH12	1:A:115:HIS:HB3	0.69	0.48
1:B:650:LEU:O	1:B:654:THR:HG23	2.13	0.48
1:C:116:VAL:O	1:C:120:VAL:HG23	2.13	0.48
1:C:650:LEU:O	1:C:654:THR:HG23	2.13	0.48
1:D:778:VAL:O	1:D:782:ILE:HG13	2.13	0.48
1:B:480:ALA:O	1:B:606:SER:CB	2.60	0.48
1:C:598:LEU:HG	1:C:611:LEU:HD21	1.95	0.48
1:D:600:ARG:HD2	1:D:1047:ASP:CG	2.39	0.48
1:A:431:LEU:HD13	1:A:526:LEU:HB3	1.92	0.48
1:B:600:ARG:HD2	1:B:1047:ASP:CG	2.39	0.48
1:A:141:SER:HA	1:A:188:VAL:HB	1.95	0.48
1:B:243:MET:O	1:B:246:ALA:HB3	2.14	0.48
1:D:964:VAL:O	1:D:968:LEU:CB	2.62	0.48
1:A:600:ARG:HD2	1:A:1047:ASP:CG	2.39	0.47
1:B:116:VAL:O	1:B:120:VAL:HG23	2.13	0.47
1:C:970:MET:HE1	1:D:970:MET:CE	2.44	0.47
1:D:243:MET:O	1:D:246:ALA:HB3	2.14	0.47
1:D:415:TYR:CE1	1:D:513:SER:CA	2.94	0.47
1:B:977:PHE:O	1:B:981:PHE:CA	2.63	0.47
1:C:431:LEU:HD13	1:C:526:LEU:HB3	1.92	0.47
1:C:977:PHE:O	1:C:981:PHE:CA	2.63	0.47
1:A:977:PHE:O	1:A:981:PHE:CA	2.63	0.47
1:A:465:SER:OG	1:A:466:LEU:N	2.46	0.47
1:A:863:ILE:O	1:A:867:ARG:HG2	2.15	0.47
1:C:546:ALA:HB2	1:C:605:TRP:CH2	2.50	0.47
1:C:600:ARG:HD2	1:C:1047:ASP:OD2	2.15	0.47
1:A:650:LEU:O	1:A:654:THR:HG23	2.13	0.47
1:D:600:ARG:HD2	1:D:1047:ASP:OD2	2.15	0.47
1:A:600:ARG:HD2	1:A:1047:ASP:OD2	2.15	0.47
1:A:984:VAL:HA	1:A:988:ALA:HB3	1.96	0.47
1:B:108:LEU:CA	1:B:178:LEU:HD13	2.44	0.47
1:B:288:LYS:HG3	1:B:289:PHE:HD1	1.80	0.47
1:B:546:ALA:HB2	1:B:605:TRP:CH2	2.50	0.47
1:B:600:ARG:HD2	1:B:1047:ASP:OD2	2.15	0.47
1:C:600:ARG:HD2	1:C:1047:ASP:CG	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:VAL:O	1:D:120:VAL:HG23	2.13	0.47
1:D:546:ALA:HB2	1:D:605:TRP:CH2	2.50	0.47
1:D:612:HIS:O	1:D:615:THR:OG1	2.30	0.47
1:D:863:ILE:O	1:D:867:ARG:HG2	2.15	0.47
1:A:546:ALA:HB2	1:A:605:TRP:CH2	2.50	0.47
1:C:991:PHE:O	1:C:995:GLN:N	2.36	0.47
1:A:108:LEU:CA	1:A:178:LEU:HD13	2.44	0.47
1:C:243:MET:O	1:C:246:ALA:HB3	2.14	0.47
1:C:1006:ARG:HG2	1:C:1007:PRO:HD2	1.97	0.47
1:D:108:LEU:CA	1:D:178:LEU:HD13	2.44	0.47
1:C:87:VAL:HG13	1:C:88:LEU:N	2.30	0.47
1:D:764:SER:O	1:D:768:VAL:HG23	2.15	0.47
1:B:1006:ARG:HG2	1:B:1007:PRO:HD2	1.97	0.46
1:C:841:PHE:O	1:C:845:THR:HG23	2.15	0.46
1:D:87:VAL:HG13	1:D:88:LEU:N	2.30	0.46
1:D:984:VAL:HA	1:D:988:ALA:HB3	1.96	0.46
1:A:841:PHE:O	1:A:845:THR:HG23	2.16	0.46
1:B:964:VAL:O	1:B:968:LEU:CB	2.64	0.46
1:B:984:VAL:HA	1:B:988:ALA:HB3	1.96	0.46
1:D:330:ASP:N	1:D:330:ASP:OD1	2.49	0.46
1:B:330:ASP:OD1	1:B:330:ASP:N	2.49	0.46
1:C:108:LEU:CA	1:C:178:LEU:HD13	2.44	0.46
1:C:288:LYS:HG3	1:C:289:PHE:HD1	1.80	0.46
1:C:793:ARG:HD2	1:C:793:ARG:HA	1.76	0.46
1:C:863:ILE:HG22	1:C:988:ALA:CB	2.39	0.46
1:C:976:MET:O	1:C:980:THR:CA	2.63	0.46
1:D:976:MET:O	1:D:980:THR:CA	2.63	0.46
1:A:87:VAL:HG13	1:A:88:LEU:N	2.30	0.46
1:A:288:LYS:HG3	1:A:289:PHE:HD1	1.80	0.46
1:A:964:VAL:O	1:A:968:LEU:CB	2.63	0.46
1:B:764:SER:O	1:B:768:VAL:HG23	2.15	0.46
1:B:863:ILE:O	1:B:867:ARG:HG2	2.15	0.46
1:C:110:VAL:HG13	1:C:110:VAL:O	2.16	0.46
1:C:648:ARG:NH1	1:C:663:LEU:O	2.49	0.46
1:D:288:LYS:HG3	1:D:289:PHE:HD1	1.80	0.46
1:D:1006:ARG:HG2	1:D:1007:PRO:HD2	1.97	0.46
1:A:330:ASP:N	1:A:330:ASP:OD1	2.48	0.46
1:A:1006:ARG:HG2	1:A:1007:PRO:HD2	1.97	0.46
1:B:984:VAL:CB	1:B:988:ALA:HB3	2.46	0.46
1:C:764:SER:O	1:C:768:VAL:HG23	2.15	0.46
1:C:984:VAL:HA	1:C:988:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:977:PHE:O	1:D:981:PHE:CA	2.63	0.46
1:A:976:MET:O	1:A:980:THR:CA	2.63	0.46
1:B:87:VAL:HG13	1:B:88:LEU:N	2.30	0.46
1:B:648:ARG:NH1	1:B:663:LEU:O	2.49	0.46
1:B:976:MET:O	1:B:980:THR:CA	2.63	0.46
1:A:984:VAL:CB	1:A:988:ALA:HB3	2.46	0.46
1:B:110:VAL:O	1:B:110:VAL:HG13	2.16	0.46
1:D:648:ARG:NH1	1:D:663:LEU:O	2.49	0.46
1:D:967:VAL:O	1:D:971:ASN:CB	2.64	0.46
1:B:967:VAL:O	1:B:971:ASN:CB	2.64	0.46
1:C:863:ILE:O	1:C:867:ARG:HG2	2.15	0.46
1:D:841:PHE:O	1:D:845:THR:HG23	2.16	0.46
1:A:484:PHE:CE1	1:A:518:ARG:CZ	2.99	0.46
1:A:764:SER:O	1:A:768:VAL:HG23	2.16	0.46
1:A:852:PHE:CE2	1:B:877:PHE:CE2	3.04	0.46
1:B:1043:PRO:HG2	1:B:1046:VAL:HG23	1.98	0.46
1:B:841:PHE:O	1:B:845:THR:HG23	2.16	0.46
1:D:110:VAL:HG13	1:D:110:VAL:O	2.16	0.46
1:D:984:VAL:CB	1:D:988:ALA:HB3	2.46	0.46
1:C:984:VAL:CB	1:C:988:ALA:HB3	2.46	0.45
1:D:583:PHE:HA	1:D:586:CYS:SG	2.57	0.45
1:A:583:PHE:HA	1:A:586:CYS:SG	2.57	0.45
1:D:863:ILE:HG22	1:D:988:ALA:CB	2.39	0.45
1:A:110:VAL:O	1:A:110:VAL:HG13	2.16	0.45
1:B:484:PHE:CE1	1:B:518:ARG:CZ	2.99	0.45
1:C:484:PHE:CE1	1:C:518:ARG:CZ	2.99	0.45
1:A:999:LEU:HD21	1:A:1003:TYR:HD2	1.82	0.45
1:C:546:ALA:C	1:C:548:LEU:H	2.25	0.45
1:D:484:PHE:CE1	1:D:518:ARG:CZ	2.99	0.45
1:D:1044:ASP:O	1:D:1048:GLN:HG3	2.16	0.45
1:A:1043:PRO:HG2	1:A:1046:VAL:HG23	1.98	0.45
1:B:480:ALA:O	1:B:605:TRP:O	2.35	0.45
1:B:999:LEU:HD21	1:B:1003:TYR:HD2	1.82	0.45
1:C:999:LEU:HD23	1:C:999:LEU:O	2.17	0.45
1:C:1043:PRO:HG2	1:C:1046:VAL:HG23	1.98	0.45
1:D:796:LYS:O	1:D:799:THR:OG1	2.26	0.45
1:A:648:ARG:NH1	1:A:663:LEU:O	2.49	0.45
1:B:105:THR:O	1:B:138:GLY:HA2	2.17	0.45
1:D:105:THR:O	1:D:138:GLY:HA2	2.17	0.45
1:B:583:PHE:HA	1:B:586:CYS:SG	2.57	0.45
1:C:424:SER:O	1:C:424:SER:OG	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:PHE:HA	1:C:586:CYS:SG	2.57	0.45
1:C:1044:ASP:O	1:C:1048:GLN:HG3	2.17	0.45
1:A:105:THR:O	1:A:138:GLY:HA2	2.17	0.45
1:A:294:PHE:HB3	1:A:299:ILE:HD11	1.99	0.45
1:A:353:ASP:OD1	1:A:353:ASP:N	2.50	0.45
1:A:1044:ASP:O	1:A:1048:GLN:HG3	2.17	0.45
1:C:294:PHE:HB3	1:C:299:ILE:HD11	1.99	0.45
1:D:480:ALA:O	1:D:605:TRP:O	2.35	0.45
1:D:999:LEU:C	1:D:999:LEU:CD2	2.85	0.45
1:D:1043:PRO:HG2	1:D:1046:VAL:HG23	1.98	0.45
1:D:999:LEU:HD23	1:D:999:LEU:O	2.17	0.45
1:B:999:LEU:HD23	1:B:999:LEU:O	2.17	0.45
1:C:999:LEU:HD21	1:C:1003:TYR:HD2	1.82	0.45
1:A:806:TRP:CE3	1:A:850:HIS:HB2	2.52	0.44
1:B:1044:ASP:O	1:B:1048:GLN:HG3	2.17	0.44
1:C:105:THR:O	1:C:138:GLY:HA2	2.17	0.44
1:C:87:VAL:HG11	1:C:321:PHE:HD2	1.83	0.44
1:C:277:VAL:O	1:C:303:THR:OG1	2.21	0.44
1:D:999:LEU:HD21	1:D:1003:TYR:HD2	1.82	0.44
1:C:784:GLN:NE2	1:C:1002:GLU:HG3	2.32	0.44
1:D:784:GLN:NE2	1:D:1002:GLU:HG3	2.32	0.44
1:B:243:MET:HG3	1:B:253:TRP:CZ2	2.53	0.44
1:B:294:PHE:HB3	1:B:299:ILE:HD11	1.99	0.44
1:D:546:ALA:C	1:D:548:LEU:H	2.25	0.44
1:A:784:GLN:NE2	1:A:1002:GLU:HG3	2.32	0.44
1:B:353:ASP:OD1	1:B:353:ASP:N	2.50	0.44
1:B:863:ILE:HG22	1:B:988:ALA:CB	2.39	0.44
1:C:480:ALA:O	1:C:605:TRP:O	2.35	0.44
1:D:243:MET:HG3	1:D:253:TRP:CZ2	2.53	0.44
1:D:277:VAL:O	1:D:303:THR:OG1	2.21	0.44
1:A:243:MET:HG3	1:A:253:TRP:CZ2	2.53	0.44
1:A:480:ALA:O	1:A:605:TRP:O	2.35	0.44
1:A:967:VAL:O	1:A:971:ASN:CB	2.66	0.44
1:B:784:GLN:NE2	1:B:1002:GLU:HG3	2.32	0.44
1:B:806:TRP:CE3	1:B:850:HIS:HB2	2.52	0.44
1:C:243:MET:HG3	1:C:253:TRP:CZ2	2.53	0.44
1:D:288:LYS:HG3	1:D:289:PHE:CD1	2.53	0.44
1:D:872:VAL:HG13	1:D:873:PHE:H	1.83	0.44
1:C:806:TRP:CE3	1:C:850:HIS:HB2	2.52	0.44
1:D:294:PHE:HB3	1:D:299:ILE:HD11	1.99	0.44
1:A:773:TRP:CZ2	1:A:1012:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:HG3	1:B:289:PHE:CD1	2.53	0.44
1:B:656:PRO:HA	1:B:659:ILE:HD12	2.00	0.44
1:C:404:ASP:OD1	1:C:404:ASP:O	2.36	0.44
1:D:111:GLY:C	1:D:113:ALA:H	2.26	0.44
1:D:656:PRO:HA	1:D:659:ILE:HD12	2.00	0.44
1:C:997:TYR:CD2	1:C:997:TYR:C	2.96	0.44
1:D:424:SER:O	1:D:424:SER:OG	2.27	0.44
1:D:806:TRP:CE3	1:D:850:HIS:HB2	2.52	0.44
1:D:833:GLY:O	1:D:837:LEU:HD13	2.18	0.44
1:A:111:GLY:C	1:A:113:ALA:H	2.26	0.43
1:A:288:LYS:HG3	1:A:289:PHE:CD1	2.53	0.43
1:A:999:LEU:HD23	1:A:999:LEU:O	2.17	0.43
1:B:87:VAL:HG11	1:B:321:PHE:HD2	1.83	0.43
1:D:1010:ALA:HB1	1:D:1011:PRO:HD2	2.01	0.43
1:A:69:VAL:HG12	1:A:229:LEU:HB3	2.01	0.43
1:A:546:ALA:C	1:A:548:LEU:H	2.25	0.43
1:B:833:GLY:O	1:B:837:LEU:HD13	2.18	0.43
1:C:612:HIS:O	1:C:615:THR:OG1	2.30	0.43
1:A:842:MET:O	1:A:845:THR:OG1	2.29	0.43
1:B:111:GLY:C	1:B:113:ALA:N	2.77	0.43
1:B:773:TRP:CZ2	1:B:1012:PRO:HG3	2.53	0.43
1:B:872:VAL:HG13	1:B:873:PHE:H	1.83	0.43
1:C:801:TYR:CE1	1:C:807:ASN:HB3	2.54	0.43
1:D:87:VAL:HG11	1:D:321:PHE:HD2	1.83	0.43
1:D:404:ASP:OD1	1:D:404:ASP:O	2.36	0.43
1:A:632:LEU:HB3	1:A:1000:ILE:HD12	2.01	0.43
1:A:656:PRO:HA	1:A:659:ILE:HD12	2.00	0.43
1:B:632:LEU:HD21	1:B:997:TYR:CD1	2.53	0.43
1:C:69:VAL:HG12	1:C:229:LEU:HB3	2.01	0.43
1:C:111:GLY:C	1:C:113:ALA:N	2.77	0.43
1:C:288:LYS:HG3	1:C:289:PHE:CD1	2.53	0.43
1:C:872:VAL:HG13	1:C:873:PHE:H	1.83	0.43
1:D:632:LEU:HD21	1:D:997:TYR:CD1	2.53	0.43
1:C:330:ASP:OD1	1:C:330:ASP:N	2.48	0.43
1:A:612:HIS:O	1:A:615:THR:OG1	2.30	0.43
1:B:1010:ALA:HB1	1:B:1011:PRO:HD2	2.01	0.43
1:A:632:LEU:HD21	1:A:997:TYR:CD1	2.53	0.43
1:B:546:ALA:C	1:B:548:LEU:H	2.25	0.43
1:C:353:ASP:OD1	1:C:353:ASP:N	2.50	0.43
1:A:87:VAL:HG11	1:A:321:PHE:HD2	1.83	0.43
1:A:404:ASP:O	1:A:404:ASP:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:C	1:B:113:ALA:H	2.26	0.43
1:C:632:LEU:HD22	1:C:1000:ILE:HD12	2.01	0.43
1:A:829:VAL:HG12	1:A:829:VAL:O	2.19	0.43
1:B:69:VAL:HG12	1:B:229:LEU:HB3	2.01	0.43
1:C:632:LEU:HD21	1:C:997:TYR:CD1	2.53	0.43
1:C:829:VAL:HG12	1:C:829:VAL:O	2.19	0.43
1:D:773:TRP:CZ2	1:D:1012:PRO:HG3	2.53	0.43
1:D:829:VAL:O	1:D:829:VAL:HG12	2.19	0.43
1:B:801:TYR:CE1	1:B:807:ASN:HB3	2.54	0.43
1:C:773:TRP:CZ2	1:C:1012:PRO:HG3	2.53	0.43
1:C:833:GLY:O	1:C:837:LEU:HD13	2.18	0.43
1:C:1010:ALA:HB1	1:C:1011:PRO:HD2	2.01	0.43
1:D:530:TYR:O	1:D:533:ALA:N	2.52	0.43
1:D:632:LEU:HB3	1:D:1000:ILE:HD12	2.00	0.43
1:A:1010:ALA:HB1	1:A:1011:PRO:HD2	2.01	0.42
1:C:656:PRO:HA	1:C:659:ILE:HD12	2.00	0.42
1:D:438:LYS:HD2	1:D:438:LYS:HA	1.85	0.42
1:A:801:TYR:CE1	1:A:807:ASN:HB3	2.54	0.42
1:B:552:LYS:HD3	1:B:617:ALA:HA	2.01	0.42
1:B:784:GLN:HE22	1:B:1002:GLU:CD	2.27	0.42
1:C:530:TYR:O	1:C:533:ALA:N	2.52	0.42
1:A:833:GLY:O	1:A:837:LEU:HD13	2.18	0.42
1:B:404:ASP:OD1	1:B:404:ASP:O	2.36	0.42
1:B:461:LEU:HA	1:B:462:PRO:HD3	1.93	0.42
1:B:796:LYS:O	1:B:799:THR:OG1	2.26	0.42
1:B:829:VAL:HG12	1:B:829:VAL:O	2.19	0.42
1:D:69:VAL:HG12	1:D:229:LEU:HB3	2.01	0.42
1:A:637:TRP:CE3	1:A:731:VAL:HG11	2.54	0.42
1:A:959:VAL:HA	1:A:962:LEU:HG	2.02	0.42
1:B:632:LEU:HB3	1:B:1000:ILE:HD12	2.00	0.42
1:B:1044:ASP:CB	1:B:1045:PRO:CD	2.98	0.42
1:D:353:ASP:N	1:D:353:ASP:OD1	2.50	0.42
1:D:637:TRP:CE3	1:D:731:VAL:HG11	2.55	0.42
1:A:530:TYR:O	1:A:533:ALA:N	2.52	0.42
1:B:997:TYR:CD2	1:B:997:TYR:C	2.96	0.42
1:D:784:GLN:HE22	1:D:1002:GLU:CD	2.27	0.42
1:A:872:VAL:HG13	1:A:873:PHE:H	1.83	0.42
1:B:637:TRP:CE3	1:B:731:VAL:HG11	2.55	0.42
1:B:999:LEU:C	1:B:999:LEU:CD2	2.85	0.42
1:D:305:LEU:HD23	1:D:305:LEU:HA	1.91	0.42
1:D:552:LYS:HD3	1:D:617:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:632:LEU:HD22	1:D:1000:ILE:HD12	2.01	0.42
1:D:1044:ASP:CB	1:D:1045:PRO:CD	2.98	0.42
1:C:632:LEU:HB3	1:C:1000:ILE:HD12	2.01	0.42
1:C:637:TRP:CE3	1:C:731:VAL:HG11	2.55	0.42
1:C:959:VAL:HA	1:C:962:LEU:HG	2.02	0.42
1:D:801:TYR:CE1	1:D:807:ASN:HB3	2.54	0.42
1:A:784:GLN:HE22	1:A:1002:GLU:CD	2.27	0.42
1:A:863:ILE:HG22	1:A:988:ALA:CB	2.39	0.42
1:C:520:LEU:HD13	1:C:536:PHE:CZ	2.55	0.42
1:C:784:GLN:HE22	1:C:1002:GLU:CD	2.27	0.42
1:A:520:LEU:HD13	1:A:536:PHE:CZ	2.55	0.42
1:A:970:MET:HE3	1:A:970:MET:HB2	1.91	0.42
1:B:520:LEU:HD13	1:B:536:PHE:CZ	2.55	0.42
1:B:862:ILE:HD12	1:B:862:ILE:H	1.85	0.42
1:C:544:VAL:HB	1:C:582:LEU:HD23	2.02	0.42
1:C:842:MET:O	1:C:845:THR:OG1	2.29	0.42
1:D:856:LYS:HA	1:D:992:TRP:CZ2	2.55	0.42
1:A:632:LEU:HD22	1:A:1000:ILE:HD12	2.01	0.42
1:A:997:TYR:CD2	1:A:997:TYR:C	2.96	0.42
1:B:438:LYS:HD2	1:B:438:LYS:HA	1.85	0.42
1:B:530:TYR:O	1:B:533:ALA:N	2.52	0.42
1:B:1077:LEU:HD23	1:B:1077:LEU:HA	1.87	0.42
1:D:544:VAL:HB	1:D:582:LEU:HD23	2.02	0.42
1:A:552:LYS:HD3	1:A:617:ALA:HA	2.01	0.41
1:A:1053:TRP:HE1	1:A:1057:GLN:HE21	1.67	0.41
1:B:576:GLU:OE1	1:B:619:ALA:HB1	2.20	0.41
1:D:520:LEU:HD13	1:D:536:PHE:CZ	2.55	0.41
1:D:813:ALA:HB1	1:D:844:PHE:CE1	2.55	0.41
1:D:859:GLY:HA3	1:D:992:TRP:CD1	2.55	0.41
1:A:415:TYR:HE1	1:A:513:SER:CA	2.30	0.41
1:A:576:GLU:OE1	1:A:619:ALA:HB1	2.20	0.41
1:A:813:ALA:HB1	1:A:844:PHE:CE1	2.55	0.41
1:B:632:LEU:HD22	1:B:1000:ILE:HD12	2.01	0.41
1:B:959:VAL:HA	1:B:962:LEU:HG	2.02	0.41
1:C:111:GLY:C	1:C:113:ALA:H	2.26	0.41
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.91	0.41
1:D:334:LEU:O	1:D:338:VAL:HG23	2.20	0.41
1:A:862:ILE:HD12	1:A:862:ILE:H	1.85	0.41
1:B:856:LYS:HA	1:B:992:TRP:CZ2	2.55	0.41
1:C:813:ALA:HB1	1:C:844:PHE:CE1	2.55	0.41
1:C:856:LYS:HA	1:C:992:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:ASP:CB	1:C:1045:PRO:CD	2.98	0.41
1:D:111:GLY:C	1:D:113:ALA:N	2.77	0.41
1:A:350:ASP:OD1	1:A:350:ASP:O	2.38	0.41
1:A:793:ARG:HD2	1:A:793:ARG:HA	1.77	0.41
1:B:350:ASP:OD1	1:B:350:ASP:O	2.38	0.41
1:B:813:ALA:HB1	1:B:844:PHE:CE1	2.56	0.41
1:B:859:GLY:HA3	1:B:992:TRP:CD1	2.55	0.41
1:B:979:TYR:O	1:B:983:VAL:N	2.50	0.41
1:C:419:GLN:HG2	1:C:423:HIS:HE1	1.85	0.41
1:C:862:ILE:HD12	1:C:862:ILE:H	1.85	0.41
1:C:979:TYR:O	1:C:983:VAL:N	2.50	0.41
1:D:350:ASP:OD1	1:D:350:ASP:O	2.38	0.41
1:A:111:GLY:C	1:A:113:ALA:N	2.77	0.41
1:A:573:ALA:HB1	1:A:575:TYR:CD2	2.56	0.41
1:B:546:ALA:C	1:B:548:LEU:N	2.78	0.41
1:B:570:MET:HE3	1:B:570:MET:HB2	1.94	0.41
1:C:476:PHE:CD1	1:C:556:GLU:HG2	2.56	0.41
1:A:856:LYS:HA	1:A:992:TRP:CZ2	2.55	0.41
1:B:1053:TRP:HE1	1:B:1057:GLN:HE21	1.67	0.41
1:C:552:LYS:HD3	1:C:617:ALA:HA	2.01	0.41
1:D:461:LEU:HA	1:D:462:PRO:HD3	1.93	0.41
1:D:576:GLU:OE1	1:D:619:ALA:HB1	2.20	0.41
1:C:999:LEU:C	1:C:999:LEU:CD2	2.85	0.41
1:A:438:LYS:HA	1:A:438:LYS:HD2	1.85	0.41
1:A:476:PHE:CD1	1:A:556:GLU:HG2	2.56	0.41
1:A:546:ALA:C	1:A:548:LEU:N	2.78	0.41
1:B:573:ALA:HB1	1:B:575:TYR:CD2	2.56	0.41
1:C:576:GLU:OE1	1:C:619:ALA:HB1	2.20	0.41
1:D:862:ILE:HD12	1:D:862:ILE:H	1.85	0.41
1:D:959:VAL:HA	1:D:962:LEU:HG	2.02	0.41
1:A:334:LEU:O	1:A:338:VAL:HG23	2.20	0.41
1:A:642:THR:OG1	1:A:643:GLY:N	2.54	0.41
1:A:1044:ASP:CB	1:A:1045:PRO:CD	2.98	0.41
1:C:334:LEU:O	1:C:338:VAL:HG23	2.20	0.41
1:C:1053:TRP:HE1	1:C:1057:GLN:HE21	1.67	0.41
1:D:179:ASP:CG	1:D:181:ASN:H	2.29	0.41
1:D:419:GLN:HG2	1:D:423:HIS:HE1	1.85	0.41
1:D:476:PHE:CD1	1:D:556:GLU:HG2	2.55	0.41
1:A:658:LEU:CB	1:A:663:LEU:HD11	2.51	0.41
1:B:476:PHE:CD1	1:B:556:GLU:HG2	2.56	0.41
1:B:842:MET:O	1:B:845:THR:OG1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:773:TRP:O	1:C:776:THR:OG1	2.34	0.41
1:A:419:GLN:HG2	1:A:423:HIS:HE1	1.85	0.40
1:A:872:VAL:HG13	1:A:873:PHE:N	2.36	0.40
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.91	0.40
1:B:872:VAL:HG13	1:B:873:PHE:N	2.36	0.40
1:D:546:ALA:C	1:D:548:LEU:N	2.78	0.40
1:A:544:VAL:HB	1:A:582:LEU:HD23	2.02	0.40
1:A:762:GLY:H	1:A:763:PRO:CD	2.35	0.40
1:B:179:ASP:CG	1:B:181:ASN:H	2.29	0.40
1:B:334:LEU:O	1:B:338:VAL:HG23	2.20	0.40
1:C:72:VAL:HG21	1:C:253:TRP:CZ3	2.56	0.40
1:C:179:ASP:CG	1:C:181:ASN:H	2.29	0.40
1:A:859:GLY:HA3	1:A:992:TRP:CD1	2.55	0.40
1:B:72:VAL:HG21	1:B:253:TRP:CZ3	2.56	0.40
1:B:544:VAL:HB	1:B:582:LEU:HD23	2.02	0.40
1:B:658:LEU:CB	1:B:663:LEU:HD11	2.51	0.40
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.91	0.40
1:A:520:LEU:HD23	1:A:520:LEU:HA	1.86	0.40
1:B:415:TYR:HE1	1:B:513:SER:CA	2.30	0.40
1:C:573:ALA:HB1	1:C:575:TYR:CD2	2.56	0.40
1:C:872:VAL:HG13	1:C:873:PHE:N	2.36	0.40
1:D:573:ALA:HB1	1:D:575:TYR:CD2	2.56	0.40
1:D:997:TYR:CD2	1:D:997:TYR:C	2.96	0.40
1:A:792:THR:H	1:A:792:THR:HG23	1.66	0.40
1:B:806:TRP:CZ3	1:B:850:HIS:HB2	2.57	0.40
1:C:350:ASP:O	1:C:350:ASP:OD1	2.38	0.40
1:C:415:TYR:HD1	1:C:511:ARG:O	2.05	0.40
1:D:72:VAL:HG21	1:D:253:TRP:CZ3	2.56	0.40
1:D:415:TYR:HD1	1:D:511:ARG:O	2.05	0.40
1:D:806:TRP:CZ3	1:D:850:HIS:HB2	2.57	0.40
1:D:872:VAL:HG13	1:D:873:PHE:N	2.36	0.40
1:D:996:ARG:HH21	1:D:1000:ILE:HD11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	895/1169 (77%)	859 (96%)	36 (4%)	0	100	100
1	B	895/1169 (77%)	859 (96%)	36 (4%)	0	100	100
1	C	895/1169 (77%)	857 (96%)	38 (4%)	0	100	100
1	D	895/1169 (77%)	858 (96%)	37 (4%)	0	100	100
All	All	3580/4676 (77%)	3433 (96%)	147 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/1009 (53%)	535 (100%)	1 (0%)	87	85
1	B	536/1009 (53%)	535 (100%)	1 (0%)	87	85
1	C	536/1009 (53%)	536 (100%)	0	100	100
1	D	536/1009 (53%)	535 (100%)	1 (0%)	87	85
All	All	2144/4036 (53%)	2141 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	597	LEU
1	B	597	LEU
1	D	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	210	HIS
1	A	439	HIS
1	A	629	GLN
1	A	784	GLN
1	A	951	ASN
1	A	982	GLN
1	A	1057	GLN
1	B	66	ASN
1	B	210	HIS
1	B	439	HIS
1	B	629	GLN
1	B	784	GLN
1	B	951	ASN
1	B	982	GLN
1	B	1057	GLN
1	C	66	ASN
1	C	210	HIS
1	C	439	HIS
1	C	629	GLN
1	C	784	GLN
1	C	951	ASN
1	C	982	GLN
1	C	1057	GLN
1	D	66	ASN
1	D	210	HIS
1	D	439	HIS
1	D	629	GLN
1	D	784	GLN
1	D	951	ASN
1	D	982	GLN
1	D	1057	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

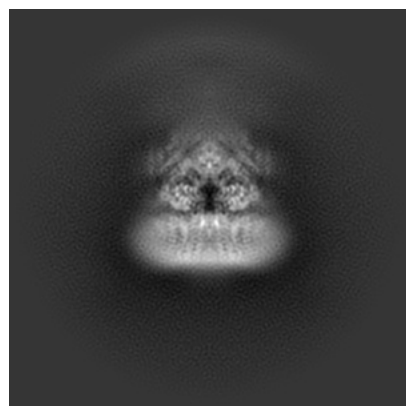
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40581. These allow visual inspection of the internal detail of the map and identification of artifacts.

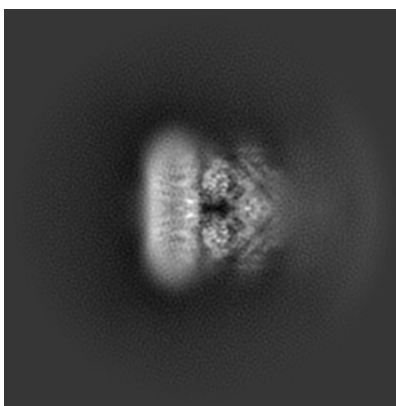
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

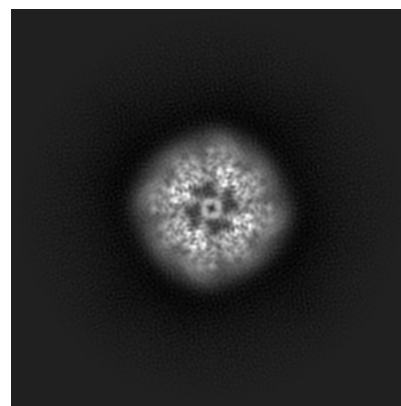
6.1.1 Primary map



X

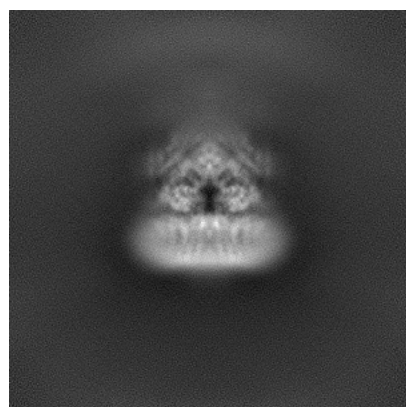


Y

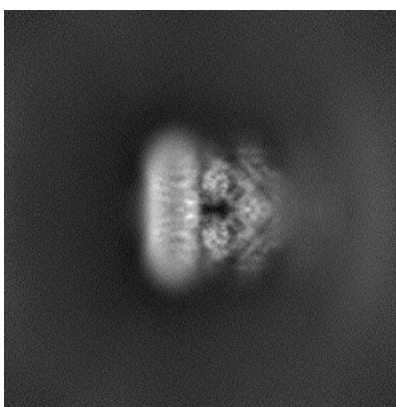


Z

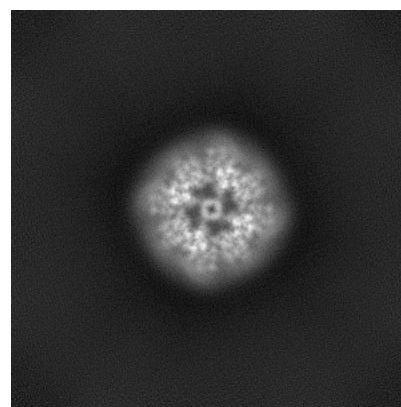
6.1.2 Raw map



X



Y

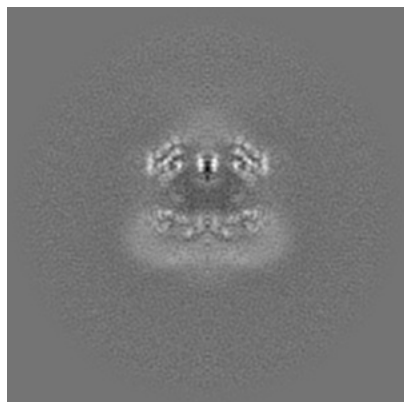


Z

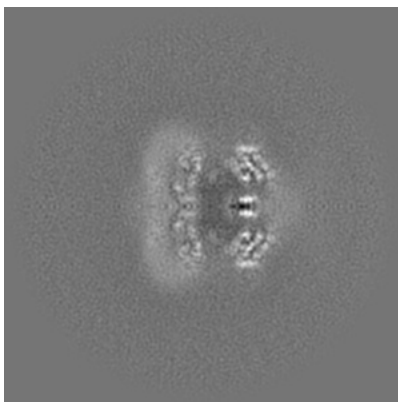
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

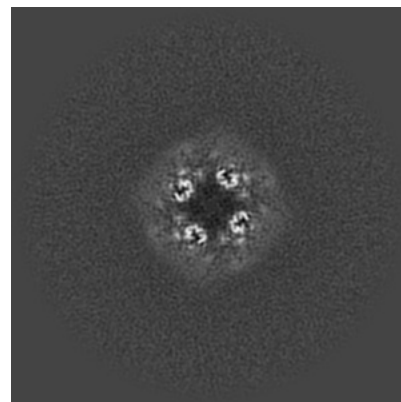
6.2.1 Primary map



X Index: 180

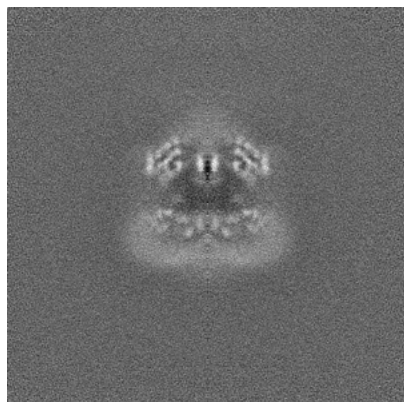


Y Index: 180

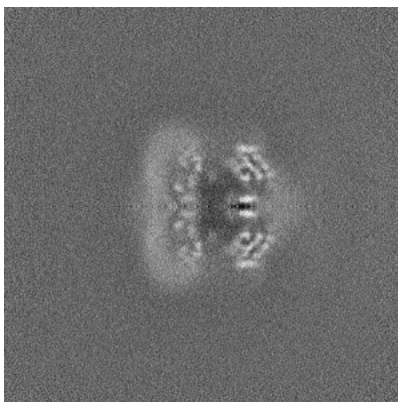


Z Index: 180

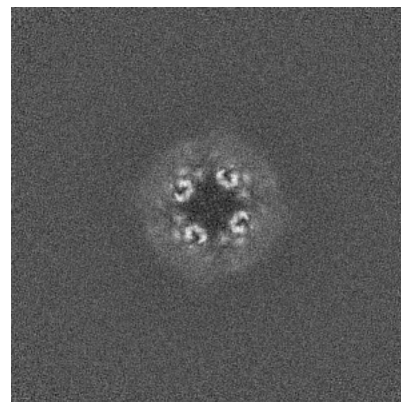
6.2.2 Raw map



X Index: 180



Y Index: 180

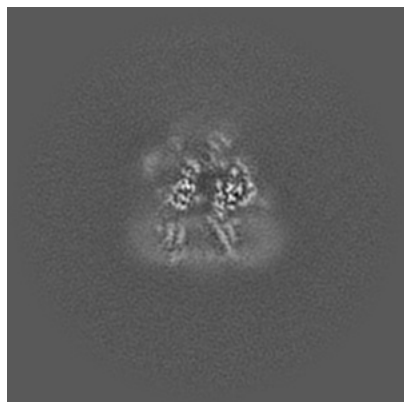


Z Index: 180

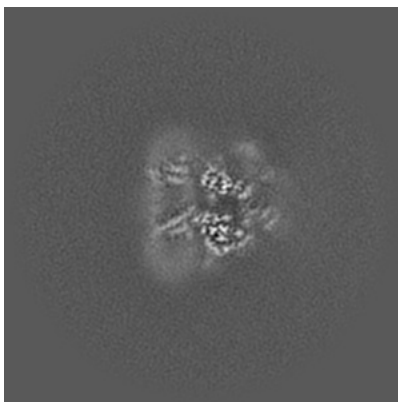
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

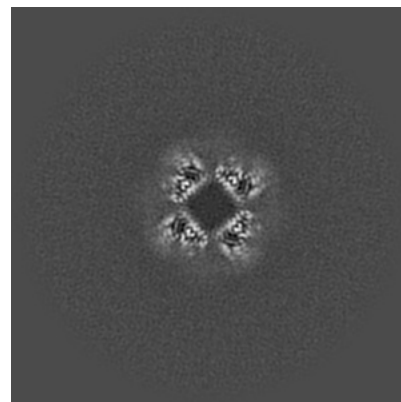
6.3.1 Primary map



X Index: 158

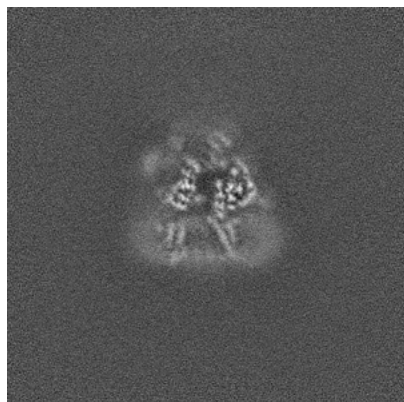


Y Index: 158

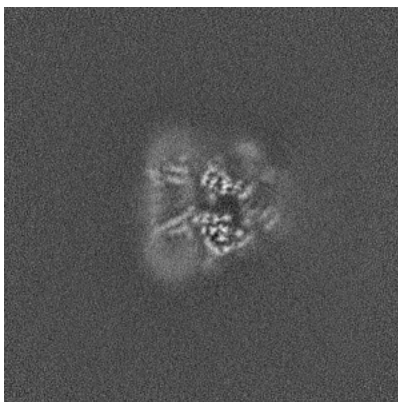


Z Index: 189

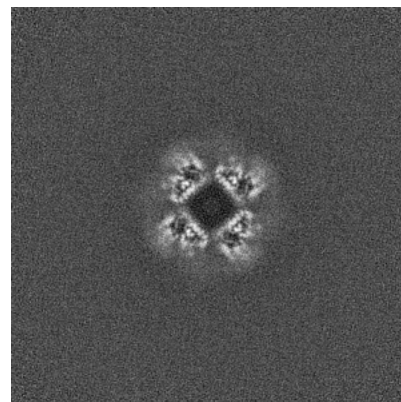
6.3.2 Raw map



X Index: 158



Y Index: 158

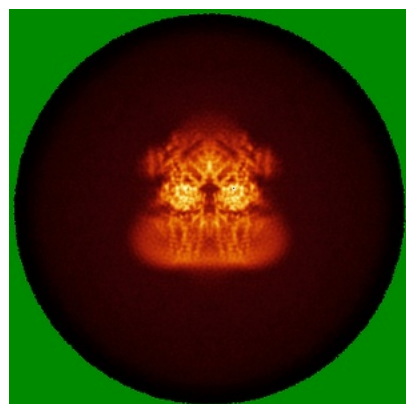


Z Index: 189

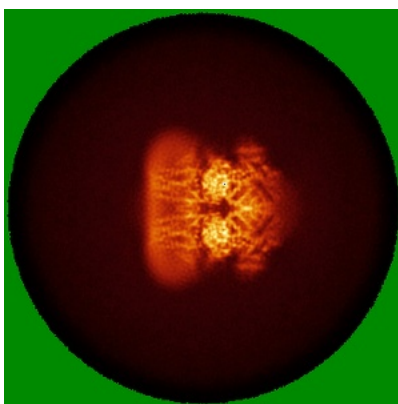
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

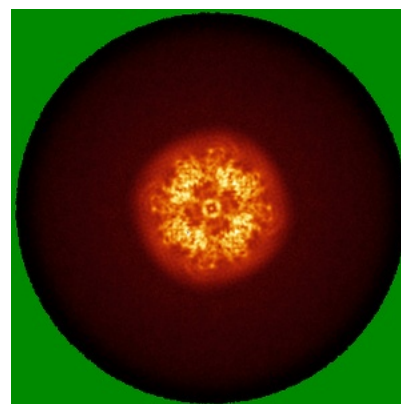
6.4.1 Primary map



X

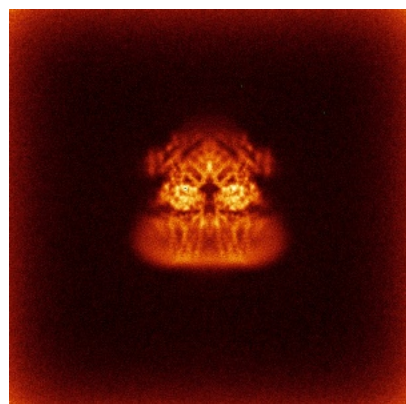


Y

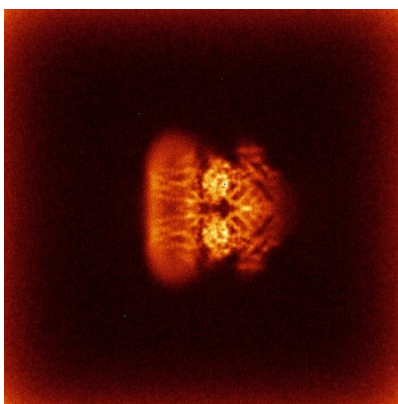


Z

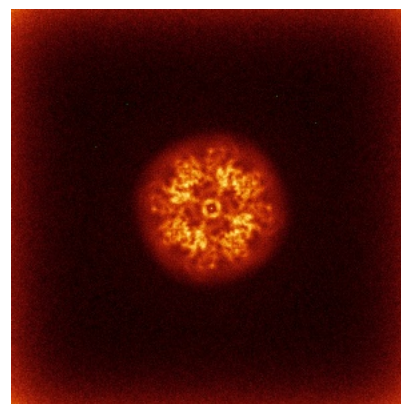
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

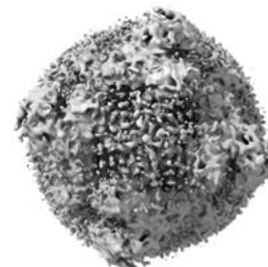
6.5.1 Primary map



X



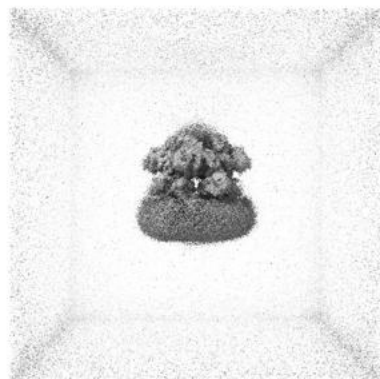
Y



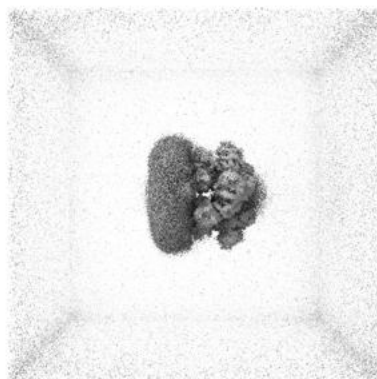
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

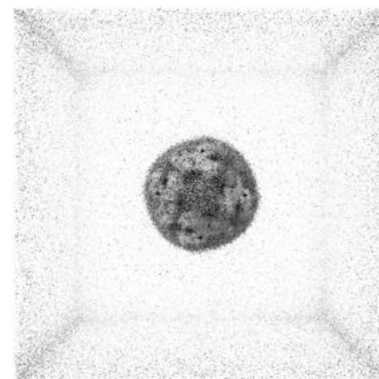
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

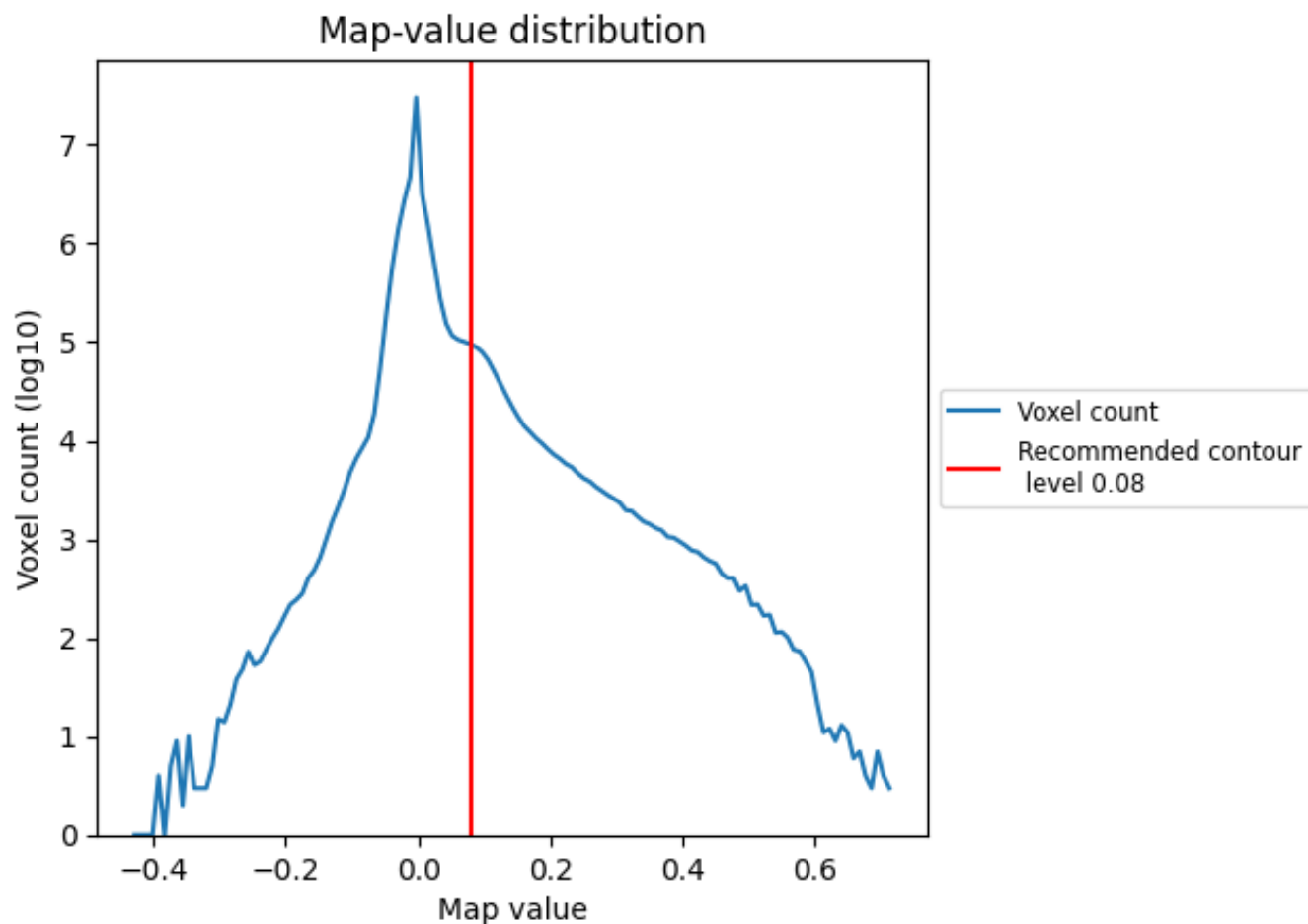
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

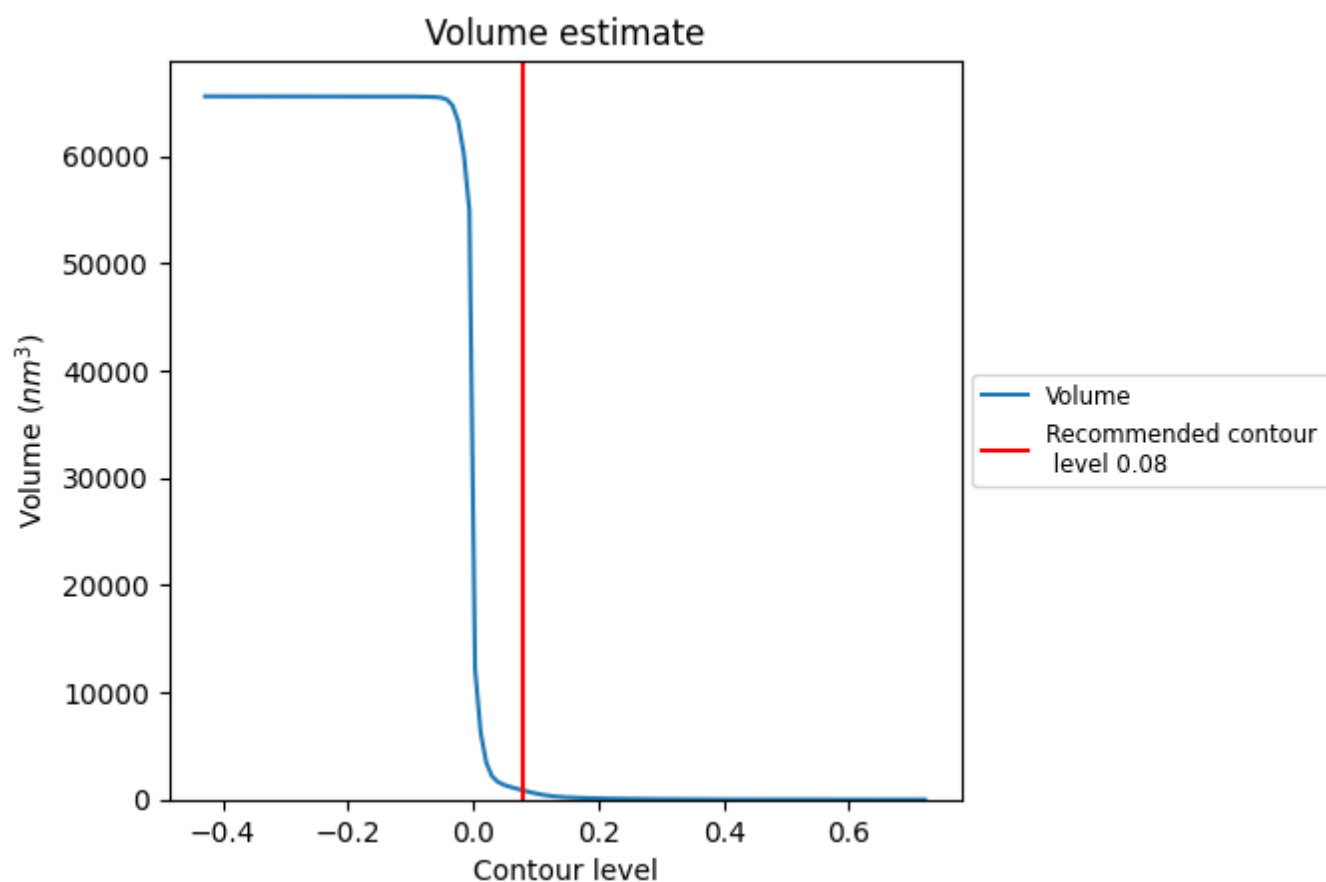
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

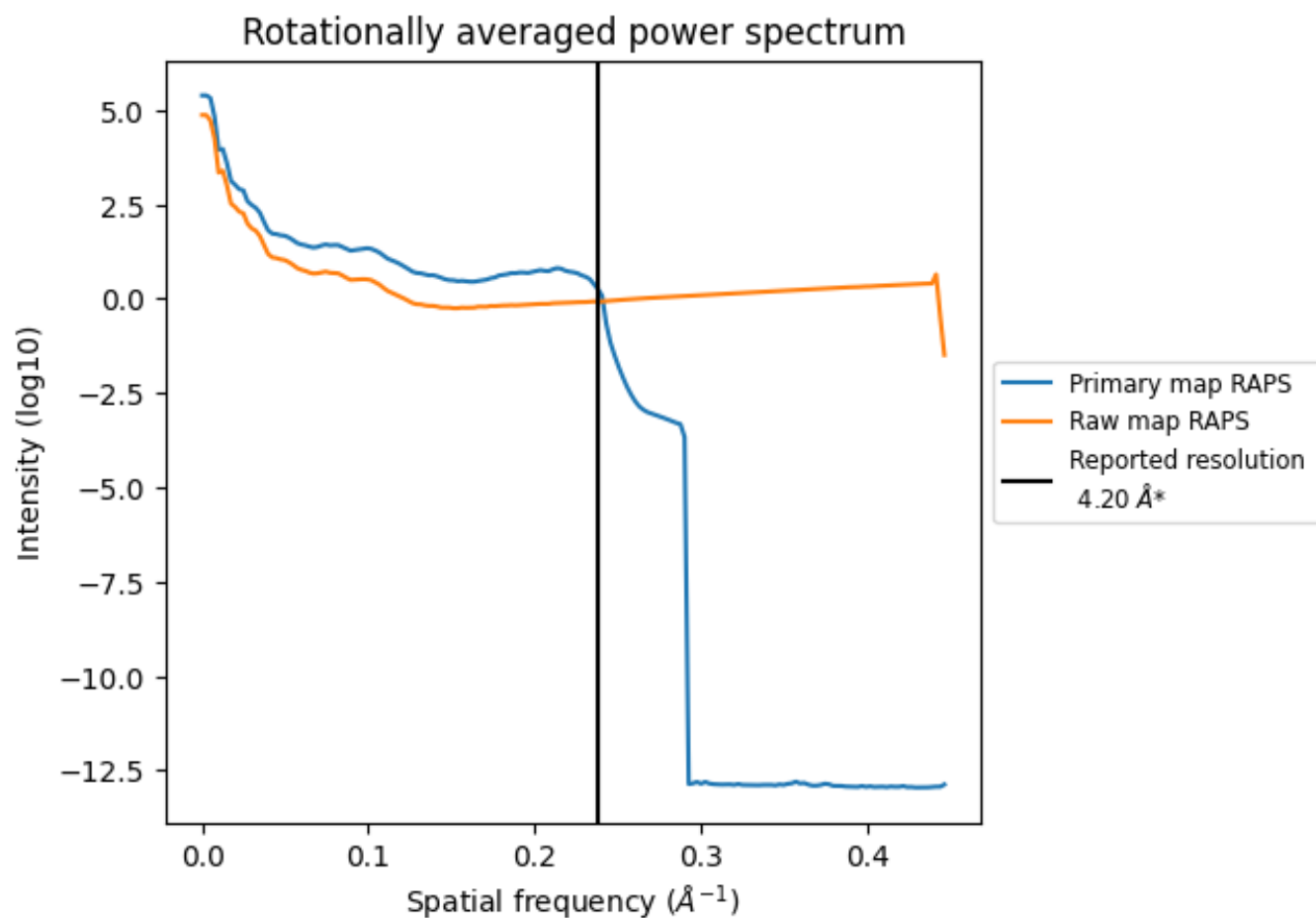
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 843 nm³; this corresponds to an approximate mass of 762 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

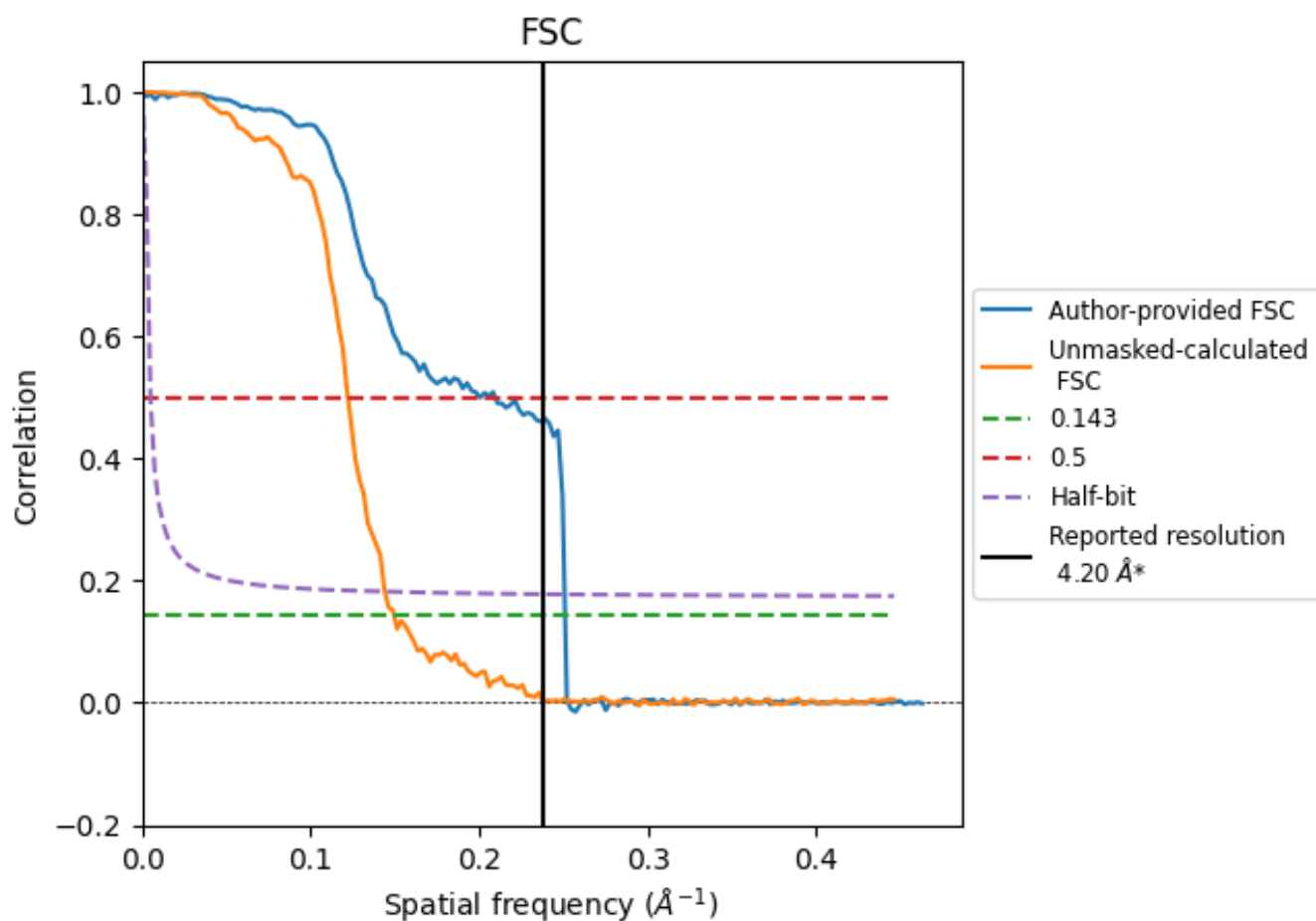


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates

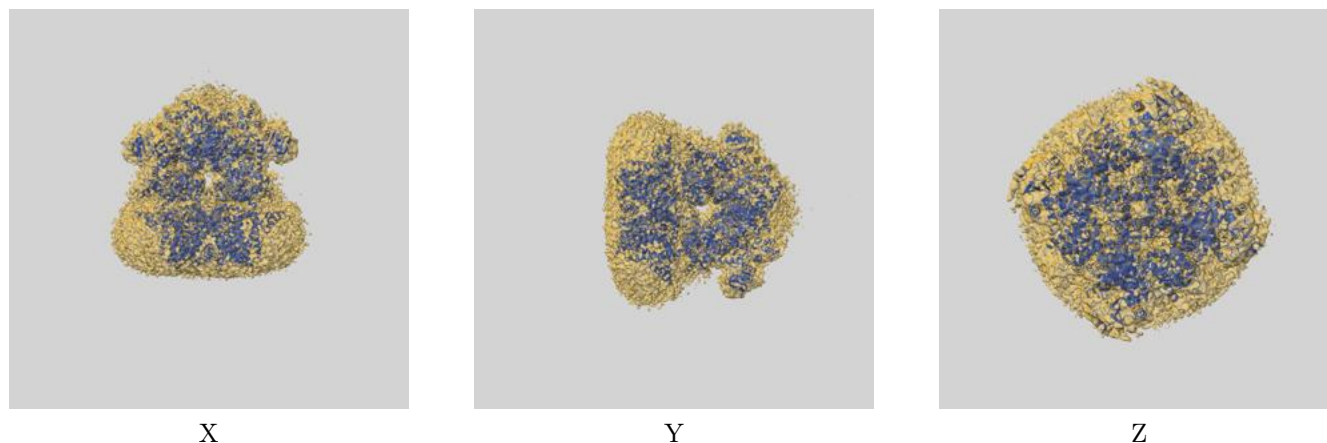
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	3.98	4.99	3.99
Unmasked-calculated*	6.69	8.19	6.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.69 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

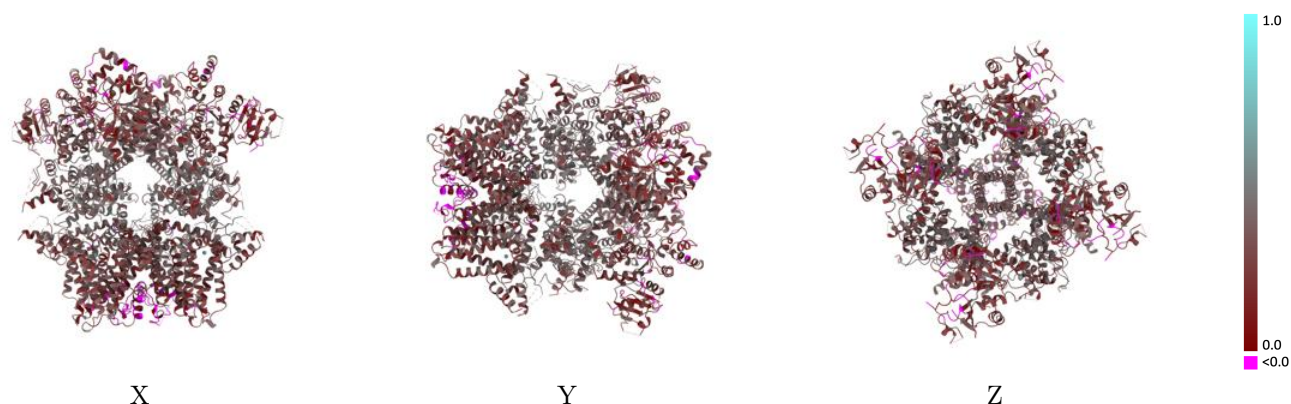
This section contains information regarding the fit between EMDB map EMD-40581 and PDB model 8SLW. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



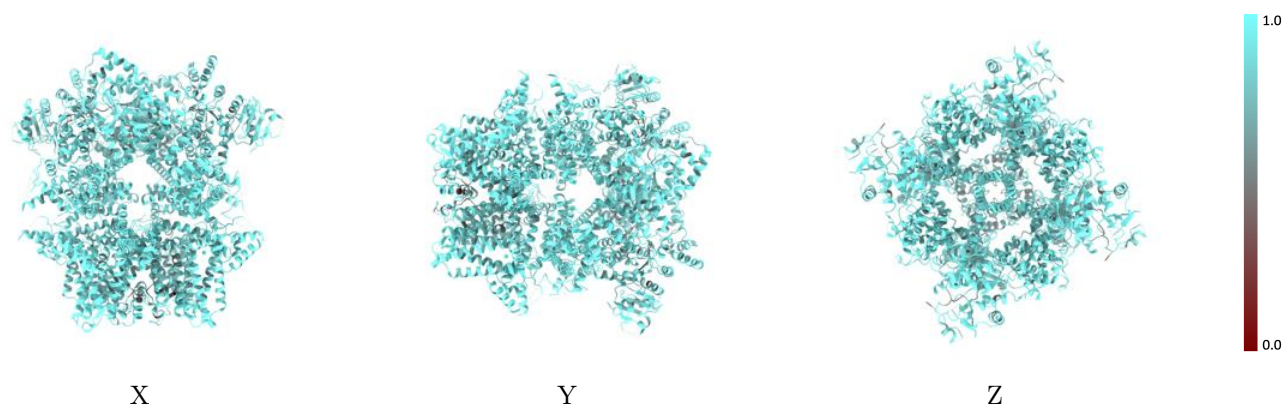
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



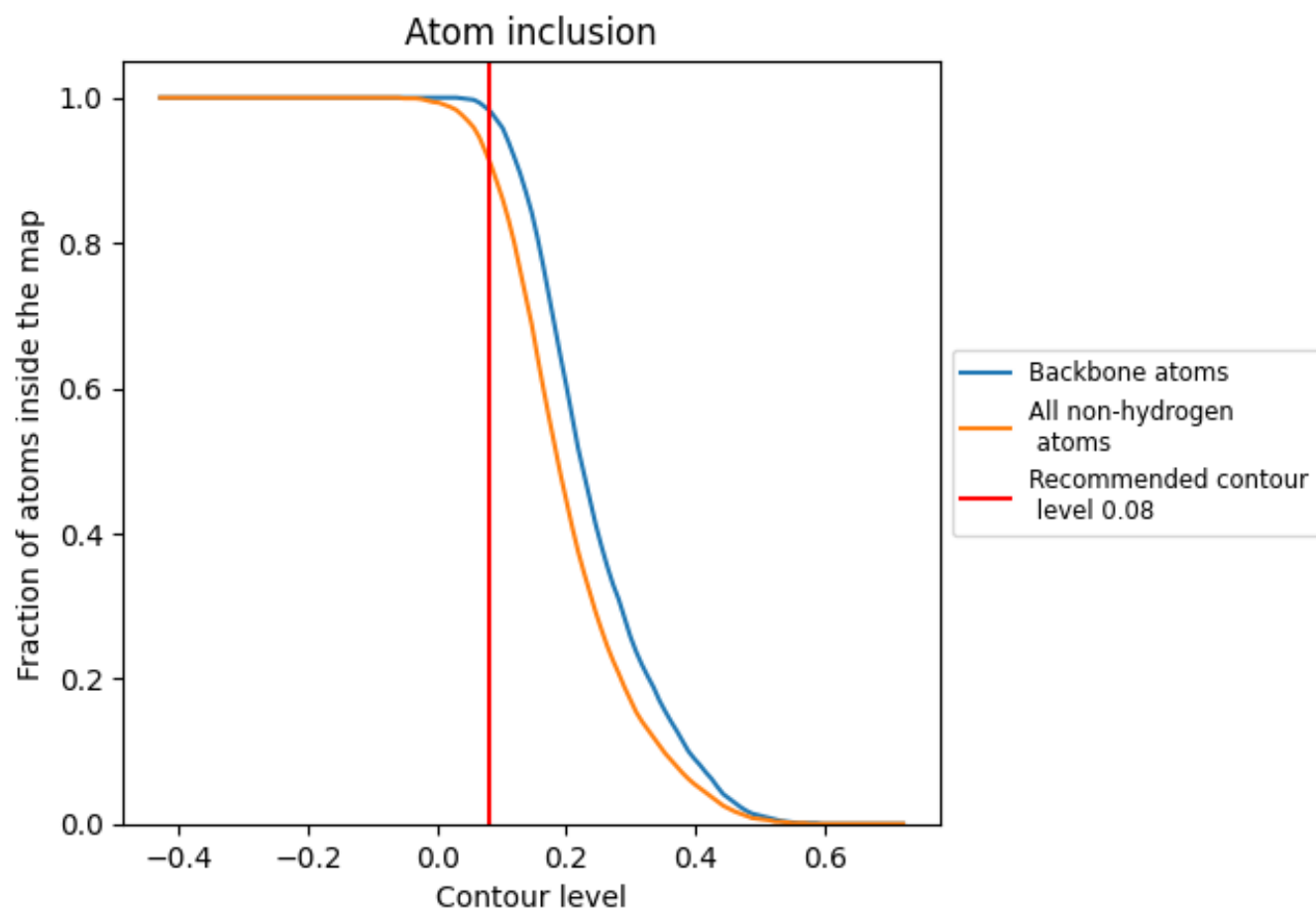
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.3060
A	0.9130	0.3050
B	0.9150	0.3060
C	0.9130	0.3070
D	0.9130	0.3070

